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REPORT

ON

STUDY OF PURE EXPLOSIVE COMPOUNDS

Part IV

Calculation of Heat of Combustion

of

Organic Compounds from Structural Features

and Calculation of Power of High Explosives

to

OFFICE OF THE CHIEF OF ORDNANCE

Contract No. DA-19-020-ORD-47

C-58247

May 1, 1952

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Arthur D. Little, Inc.

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DEPARTMENT OF THE ARMY
Boston Ordnance District
Army Base
Boston 10, Mass.

SUBJECT: "Fundamental Research on High Explosives. Part IV."
Prepared by Arthur D. Little, Inc., under Contract
DA-19-020-ORD-47

TO:

Attention:

1. You are furnished herewith Part IV of "Fundamental Research on High Explosives". This is the fourth of a series of reports prepared by Arthur D. Little, Inc., under a contract with the Ordnance Department comprising research and development in the field of military explosives.

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FOR THE DISTRICT CHIEF:

A. C. Yoksas

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Arthur D. Little, Inc.

RESEARCH · ENGINEERING · INVESTIGATION

CAMBRIDGE 42, MASSACHUSETTS

Office of the Chief of Ordnance
Pentagon Building
Washington 25, D.C.

Contract No. DA-19-020-ORD-47
C-58247

Gentlemen:

We are transmitting herewith Part IV, "Calculation of Heat of Combustion of Organic Compounds from Structural Features and Calculation of Power of High Explosives", continuing our fundamental study of explosives under the subject contract. In the earlier parts of this report we developed approximate methods for predicting performance in certain explosive tests from the concepts of oxygen balance and plosophoric groups, and from heat of explosion. These approximations were shown to be useful for both pure explosives and mixed explosives.

In the first section of this report a method for calculating heats of combustion of organic compounds, and hence heats of explosion, from structural features alone has been developed. The method is based entirely on observed heats of combustion for both explosive and non-explosive organic compounds. It represents a distinct improvement over the calculation method presented in Part II, and possesses several features which make it more adaptable and suited for our purposes than other methods proposed in the literature.

The second section of this report demonstrates the application of a system for predicting the power of an explosive, relative to TNT (or to any other substance). A comparison is made between the calculated power based on calculated heat of combustion, and the power observed in the ballistic mortar for pure compounds and for mixtures, both metallized and non-metallized. This method of prediction results in an accuracy much improved over the use of the previous concepts given in Parts I and III.

Recommendations are made for experimental work to confirm and expand the conclusions reached by this treatise.

Respectfully submitted,

Arthur D. Little, Inc.

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SUMMARY

This report describes a new method for calculating heats of combustion of explosives and non-explosive organic compounds and a method for calculating relative powers of explosive compounds from heats of combustion.

It is shown that a straight-line relationship exists between molar heat of combustion (Q_C) and molar oxygen balance for a large number of homologous series of organic compounds. From the slope and intercept coefficients of the straight lines obtained from observed data a method has been devised for calculating the heat of combustion at constant pressure (water liquid) of an organic compound, considering only the structural features of the molecule. Simple rules and examples of use are explained. The agreement between calculated and observed heat of combustion is generally better than 1%, although the variability is more pronounced with members of homologous series whose determinations are known with less assurance of accuracy.

It is shown that the coefficients of the equations can be used as a measure of the relative desirability of any functional group in an explosive compound. The coefficients have been arranged to give a quantitative idea of the energy contribution of any functional group in a molecule, based on the paraffin hydrocarbon as the zero energy potential. This means that the potentialities of a functional type can be assessed for explosive usefulness without necessity of preparing oxygen balanced compounds. Instead, an approximation can be made from a small number of organic substances containing the functional group of interest, but not necessarily any primary plosophoric group, thus eliminating the synthetic difficulties and attendant danger usually encountered

with oxygen balanced molecules. After the potentialities of the group have been determined, it can then be decided whether the effort to prepare balanced explosives is worthwhile.

This system of calculation is compared with methods proposed by others. A historical section dealing with published heats of combustion completes the presentation of this subject matter.

The relative power of an explosive compound can be calculated from its heat of combustion by an iteration method employing the estimated temperature and the moles of gas produced in the detonation. The resulting figure (= nRT) compared to the value for TNT is equal to the power of the explosive as measured in the ballistic mortar or in the spherical lead block on an equivalent weight basis. A comparison of results with more than 100 pure compounds and more than 50 organic mixtures is in agreement with this conclusion. Greater harmony is achieved if the calculated rather than observed heat of combustion is used.

The results with a large number of metallized mixtures, while not giving as close agreement as the non-metallized substances do, show that the use of nRT to predict power for this type of mixture is definitely superior to the use of the concepts of oxygen balance or heat of explosion alone, as described in Part III of this report.

The nRT method, combined with the method for calculating heat of combustion can be used to predict the expected power, as it might be measured in the ballistic mortar compared to a standard explosive, of any organic compound or mixture whose structural features are known or postulated. A quantitative arrangement of the many types of functional groups from the viewpoint of power

contribution in an explosive compound or mixture can also be obtained from use of this method for calculating power.

Thus, prior to synthesis, it can be determined with some degree of accuracy whether the effort to prepare oxygen balanced explosives containing any given functional type is worthwhile, and what functional types or mixtures might be expected to produce better power performance than the existing most powerful organic explosives.

RECOMMENDATIONS

1. Determination of the contribution to heat of combustion and explosion has been recommended for the nitroso group and for the following functional types of interest to the explosives program but not treated in this report:

azide

1,2,3-triazole and 1,2,4-triazole

furoxan and furazan

triazene, tetrazene, and other linear nitrogen chains

azine

hydrazone

imide

s-triazine

imine or anil

hydroxylamine

nitrite

perchlorate ester

2. For general interest the contribution of the following groups should be estimated:

thiol

sulfide

disulfide

sulfonic acid

chloro

bromo

iodo

isocyanate

peroxide

3. Heat of combustion should be redetermined for 2,4,6-trinitroresorcinol (styphnic acid) and for α,α,α-trifluoro-3,5-dinitrotoluene. 5-Nitraminotetrazole should be measured for heat of combustion.

None of the specific compounds and mixtures of negative oxygen balance whose observed powers are widely different from calculation are recommended for redetermination. Their low theoretical powers make them basically of no interest to a project endeavoring to improve on the present service explosives. Recommendations are made for a program of testing metalized mixtures containing high nitrogen compounds expected to have exceptionally high power, for testing certain high energy compounds, and for retesting certain substances of positive oxygen balance, such as hexanitroethane, which appear to disagree with the general theory of power calculated by nRT.

SECTION XVI
Calculation of Heats of Combustion of Organic Compounds

A. Abstract

A method of calculating heats of combustion of organic compounds from structural features is described. This method depends on the straight line relationship between molar oxygen balance and the molar heat of combustion of a homologous series. Intercept and slope values have been determined from published data for thirty-eight structural features. On the average, an accuracy of 1% is found by comparison of observed with calculated heats of combustion. The usefulness of the method for high explosives is illustrated and certain rules of procedure have been established.

B. Introduction

In an earlier report (70) a method of additive group energies was proposed for calculating heats of combustion of explosive compounds. This method was converted from the Springall and Roberts system of calculating heats of formation (130). Calculation gave good agreement with observation in most cases for organic compounds containing primary plosophoric groups (69) but it was later discovered that very poor agreement was frequently being obtained with non-explosive organic compounds whose observed values were undoubtedly correct. This poor agreement, as well as the lack of values for certain common structural features, led to a reexamination of the problem from a more empirical and less theoretical viewpoint than that of Springall and Roberts.

C. Discussion

1. Comparison with Other Methods

Holcomb et al described a relation between oxygen balance and heat of combustion on a weight basis for nitroalkanes (44) and later for nitroalcohols (31a). We have found that a similar relationship is applicable to a great many more functional types. The relationship is found to give a better straight line, however, between molar oxygen balance and molar heat of combustion, than between these parameters on a weight basis. Indeed such a weight relation does not exist for molecules with the empirical formula C_nH_{2n}. Olefins and cyclic paraffins all have the same oxygen balance on a weight basis (-342.2) and the weight heat of combustion becomes independent of this parameter. It was discovered subsequently that relationships between the molar heat of combustion and the number of carbon atoms in the molecule had been published by several investigators (11, 65, 100, 103, 113, 144, 146, and 148). None of them, though, had been or could be applied to any molecules containing more than a single type of functional group, and they were straight lines in any homologous series only above five carbon atoms.

Relating the heat of combustion to the number of carbon atoms is neither as effective nor as flexible as relating it to the molar oxygen balance which is done here for the first time. When one considers that numerous polyhomofunctional compounds can have the same number of carbon atoms but different heats of combustion, necessitating an equation for each homologous series, it is apparent that the task is simplified by use of oxygen balance which leads to a single equation for any homofunctional type regardless of the number of like functional groups present.

The method of Kharasch (55) is as close as any to the system described in this report. Yet the difficulties in calculating the number of electrons in a molecule are definitely greater than in computing the oxygen balance, a figure which can be obtained from the molecular formula alone, independent of electronic structure. Furthermore new corrections to be found for functional types not given by Kharasch are difficult to assign and assess with any assurance of accuracy (1). His method of derivation does not involve the straight line relationship which smooths out errors as it does in the system described below.

The system presented here has one distinct advantage over all previously used methods. The linearity of Q_c for any homologous series with molar oxygen balance allows a reasonable estimation of the accuracy of any reported heat of combustion. Isolated points which do not fall on the best line or within a reasonable range of it arouse suspicion of inaccurate determination for one reason or another. The truthfulness of this statement has been upheld and justified by a number of instances in the pertinent field of explosive chemistry, in which a determination, discarded by us as being incorrect, has been revised by later determination or by other authors, bringing the observed heat of combustion in line with the calculated value. An example of similar reasoning applied to structure proof can be found in the recent literature (72). Thus many of the data in the Tables 61 through 134 show the effects of some selection, and the points chosen for estimating the best line by the least squares method have been biased, but only for this reason.

The list of functional groups used may be considered incomplete. Additions will be made and reported at a future time. It may be that improved accuracy can be attained by reworking the accumulated data in a different fashion and employing punched card machine methods for this reevaluation. Such a possibility is under consideration.

2. Congruence of Observation and Calculation

The agreement between observation and calculation by the present system is generally within 1% or better, depending somewhat on the accuracy of the original data. Other factors affecting the agreement and not taken into complete consideration in deriving the equations, are effect of positional isomerism, effect of neighboring groups and branching, and effect of not taking

into account minor corrections necessary to convert observed data to a uniform basis of temperature, in vacuo measurements, Washburn corrections, and the like. It has not seemed worthwhile to make all adjustments possible because the unknown accuracy of the original data, with a few exceptions, did not warrant the effort. The data used for this study and the resulting equations are given in Tables 61-136.

There is almost perfect agreement between calculated heats of combustion and observed values for normal paraffins and certain other hydrocarbons where the data are known with considerable accuracy (115). These data are taken as the basis for the whole system which follows. For other types of functional groups the agreement is less good but satisfactory enough for the purpose intended. A graphic illustration of some of the results is given in Figure 79. The accuracy and precision of results apparently depend only on the reliability and accuracy of combustion data actually measured. The greatest deviation from the straight line relation is generally exhibited by the lowest member, and this is particularly true for the polar type of compound without carbon-carbon bonds, e.g., methanol, formic acid, formaldehyde, methylamine, and tetranitromethane.

It may be argued that the calculation method devised and reported here does not give sufficient accuracy to the heat of combustion. It seems to be adequate, however, for the purpose intended, i.e., approximation of properties of new or unknown compounds, particularly for prediction of power. In the second section of this report it is shown how well such calculated values serve to relate power as computed by the nRT product directly to power as measured in the ballistic mortar. Indeed, in a number of instances the calculated heat of combustion leads to better agreement than does observed heat of combustion. At any rate the roughness of prediction is not so great but what satisfaction can be expected when used in the field of propellants and high explosives.

3. Relationship among Functional Groups

This system of estimating heats of combustion was devised specifically for use with high explosive materials, many of which contain groups not susceptible to estimation by any other simple system. The system as presented at this time, nevertheless, can be used for any compound containing the functional groups given in Table 60. Conceivably there is no limit to the number or types of groups or bonds which can eventually be included. The present method is not claimed to be indisputable, for there exist anomalies and difficulties still to be corrected. These may be accounted for if interactions could be completely estimated.

One use to which the equation coefficients can be put is establishing the relative contribution of any functional group to heat of combustion. The same contribution will be made to heat of explosion if the point of comparison is chosen to be zero oxygen balance to carbon dioxide and water, since at this point and at positive balance these two heat quantities are identical. Moreover, at the zero point the power of pure explosive compounds, a parameter which is of vital interest to the present investigation, is at the maximum.

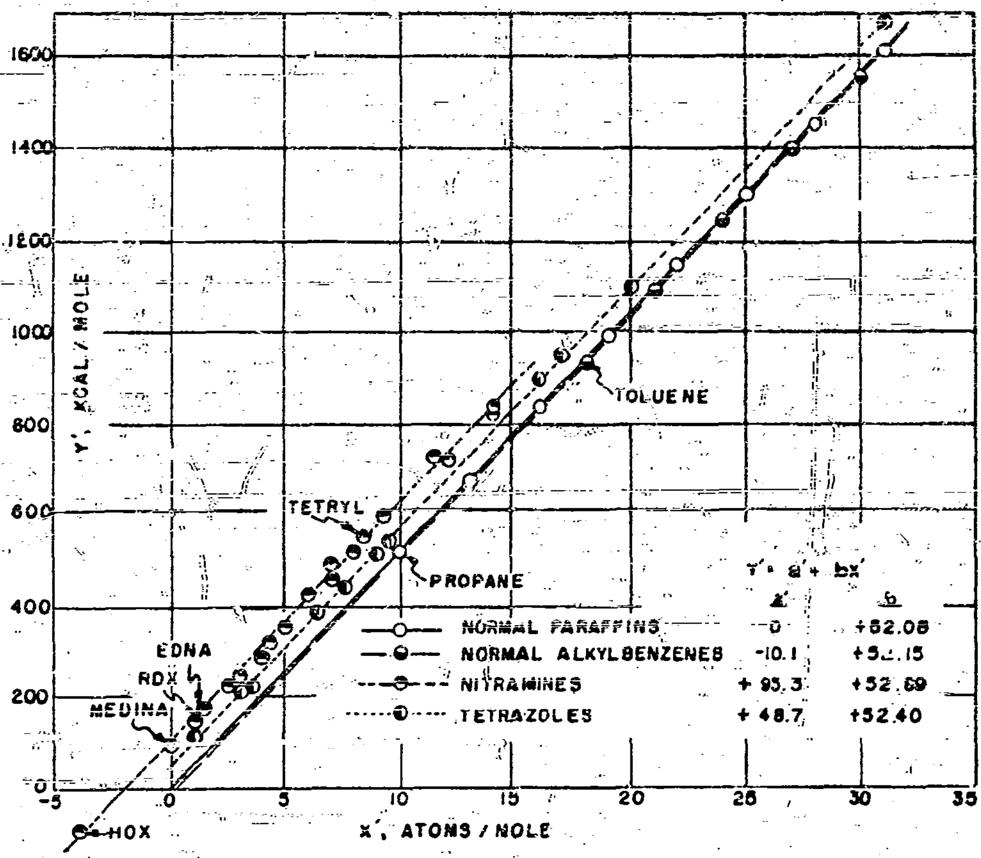


FIGURE 79
REDUCED HEAT OF COMBUSTION (Y)
VS
OXYGEN NEEDED (x)

Thus there can be constructed what might be called a "plosomotive" series to interrelate the relative desirability of a functional group in an explosive molecule. Paraffin is taken as the zero potential. The complete series is given i. Table 58. Where possible or practical the values have been listed for the liquid state, and only the most reliable or highest value for types with positional isomerism is given.

TABLE 58

PLOSOMOTIVE SERIES

Contribution of Functional Groups to Heat of Combustion

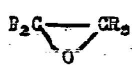
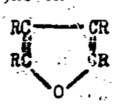
Functional Type		Contribution kcal/mole
(R=aliphatic residue or hydrogen)		
Nitrate	$RONO_2$	129
Substituted nitramide	$RC(=O)NRNO_2$	120
Secondary nitramine	R_2NNO_2	113
Primary nitramine	$RNHNO_2$	112
Nitramide	$RC(=O)\underset{\mid}{N}NO_2$	103*
Nitramine	$-\underset{\mid}{N}NO_2$	95*
Nitro	RNO_2	93
Primary nitrosamine	$RNHNO$	73
Azo compound	$RN=NR$	69
Azoxy compound		69
Hydrazine, disubstituted	$RNHNHR$	67
Nitrosamine	$-\underset{\mid}{N}NO$	56
Hydrazine, monosubstituted	$RNHNH_2$	50
Tetrazole		49
Hydrazide, monosubstituted	$RC(=O)NHNHR$	47
Oxime	$R=NOH$	45
Oxirane		41
Acetylene	$RC\equiv CR$	37
Furan		36
Azo bond-group	$-N=N-$	35*

TABLE 58 (cont'd)

PI[illegible]MOTIVE SERIES

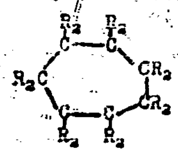
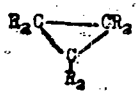
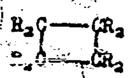
Functional Type		Contribution kcal/mole
Azoxy bond-group	$-\underset{\downarrow O}{N}=N-$	35*
Guanidine, disubstituted	RNHC(=NH)NHR	35
Hydrazine bond-group	-N-N-	33*
Hydrazide bond-group	RC(=O)N-N-	30
Carbylamine (isonitrile)	RNC	27
Thiophene		22
Nitroso	RNO	21
Guanidine, monosubstituted	RNHC(=NH)NH_2	18
Amine	RNH_2	18
Cycloheptane		17
Cyclopropane		16
Ester	RC(=O)OR	16
Ether	ROR	16
Fluorine	RF	14
Olefin	$R_2C=CR_2$	14
Aldehyde	RCHO	12
Amide, substituted	RC(=O)NHR	11
Cyclobutane		10
Alcohol	ROH	9
Nitrile	RCN	9

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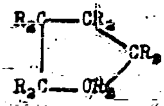
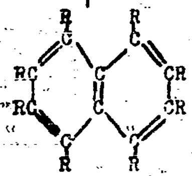
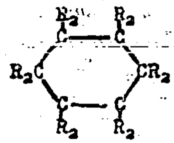
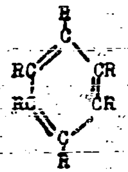
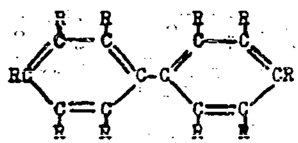
TABLE 58 (cont'd)

PLOSOMOTIVE SERIES

Functional Type		Contribution kcal/mole
Ketone	RC(=O)R	6
Acid anhydride	RC(=O)OC(=O)R	2
Guanidine	-NC(=NH)N-	1*
PARAFFIN	R-R	0
Cyclopentane		-2
Acid	RCOOH	-5
Amido	RC(=O)N-	-6*
Naphthalene		-6
Cyclohexane		-7
Benzene		-10
Salt		-16
Biphenyl		-31

*For compounds with substituents on nitrogen, add appropriate group value. For example, primary nitramine, $RNHNO_2$, contribution becomes 112.

The functional group which makes the best plosophore is the nitro group ($-NO_2$) and this attached to oxygen, nitrogen, or carbon appears highest on the list (93-129 kcal/mole). Nitrosamine (-NNO) is also high (56 kcal/mole), consistent with its secondary plosophoric nature. Nitroso (-NO, 21 kcal/mole) appears considerably lower in the scale than would be expected. This may be due to the lack of sufficient data to give a completely reliable constant, and it is reflected in the unusually high slope for this functional type (see Tables 60 and 136). Aromatic rings, unsubstituted amides, and acids appear below paraffins (-31 to -5 kcal/mole) and are not desirable for contributing to heat of explosion or combustion. Energy is added to a molecule by replacing a single bond with a double bond (olefin, 14 kcal/mole) or with a triple bond (acetylene, 37 kcal/mole). Compounds with hydrazine, azo, and azoxy groups (67-69 kcal/mole) are rich in energy and, in addition, are high in nitrogen acting as a source of extra gas volume for power, all other factors being constant. The presence of such common groups as ether, alcohol, amine, fluorine, substituted guanidine, and ester (14-18 kcal/mole) is helpful rather than detrimental. Tetrazole (49 kcal/mole) is not as good as might be expected, probably because of loss of energy due to resonance, although it can still be classed as a secondary plosophore. The same loss of energy is shown by benzene which, without resonance, ought to have been the equivalent of three olefinic bonds (42 kcal vs -10 kcal). Furan (36 kcal/mole) is not quite the sum of an ether and two double bonds (44 kcal/mole) perhaps for the same reason. Indeed, from such considerations a resonance energy value can be calculated. For the benzene ring it would amount to 52 kcal/mole and to 76 kcal/mole for naphthalene, in reasonable agreement with Wheland's assigned values of 41-51 kcal/mole and 77-86 kcal/mole respectively (151).

A table similar to Table 58 drawn up on a weight basis would be even more helpful in group evaluation from an explosive viewpoint, because of the dependence on weight rather than molar values for measuring explosive properties. Such a table can be constructed from the data on a molar basis and will be presented at a future time.

The contribution made by functional groups, as produced by the present report, converted to values which atom to atom bonds might contribute would be akin to the Pauling system of additive bond energies for heat of formation, and to the Arthur D. Little, Inc., method for heat of combustion (70), predecessor of this one. Some efforts in this direction have shown that this can be done. The conversion is easily made from the intercept and slope values shown in Table 60, but the results are not yet in a state for publication.

4. Multiple Groups on a Single Carbon Atom

Attention is drawn to another point of interest. More than one of certain groups or atoms, such as nitro or halogen, can replace the hydrogen atoms on a single carbon atom. It has been found that compounds containing such a multiplicity of function make an energy contribution to heat of combustion greater than would be expected from simple addition using the values for one function per carbon as described by the system herein. Accordingly,

special equations have been determined for the gem trinitro $[RC(NO_2)_3]$ and gem trifluoro (RCF_3) groupings. The increase for the gem tri substitution over the sum of three single groups is small (0.7% and 1% for trinitro and trifluoro, respectively). It might be attributed to the lack of hydrogen atoms for bonding which normally consume some energy, or to the energy of strain from increased bond length caused by repulsion of multiply highly electronegative groups on the same carbon atom.

The difference between the value for gem dinitro $[R_2C(NO_2)_2]$ and the sum of two mononitro (R_3CNO_2) groups was so small that it could not be determined whether it was a real difference or due to errors in experimental measurement. A separate value for gem dinitro is not included, therefore, in Table 60. From the preliminary evaluation of the enhancement effect of multiple substitution during the early stage of study on the heat of combustion problem a much larger effect for both gem di- and tri- substitution was deduced. These original conclusions have been discarded now in favor of the present more satisfactory equations.

D. Conclusions

From the evidence given in this report it is concluded that the method of calculating heat of combustion from a straight line relationship with molar oxygen balance is valid and exceedingly useful. Of the many hundreds of compounds considered the only ones of interest which are in disagreement with calculation greater than 10% are the following:

	% difference from calcn.
Tetranitromethane	+44
α,α,α-trifluoro-3,5-dinitrotoluene	-31
2-nitroethanol nitrate	-20
[illegible]	[illegible]
N-picryldiethanolamine dinitrate	+17
trinitroacetonitrile	+16
allylpentaerythritol trinitrate polymer	-12
pentanitroaniline	+11

Tetranitromethane has recently been determined with great accuracy by the National Bureau of Standards (83). It must be assumed that this compound is unique and does not fit the general scheme of the calculation method. Trifluoro-3,5-dinitrotoluene is sufficiently divergent to cast suspicion on the identity of the compound measured and should be reevaluated.

2,4,6-Trinitroresorcinol (styphnic acid) is only 3% less than calculated, and 5-nitraminotetrazole has never been measured, but current interest makes determination of both these desirable.

It thus becomes possible with this system to evaluate and screen functional groups for suitability in explosive compounds by using a limited number of non-explosive, even poorly balanced, compounds without the necessity and danger of preparing well-balanced explosives for actual testing. If any functional type is found desirable, then greater expenditure of effort can be made to prepare balanced compounds by introducing primary plosophoric groups.

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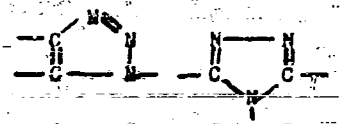
The present list of functional groups should be extended, partly for particular use with explosive compounds and partly for general use in other fields of science. The coefficients of many of them can be approximated from existing data. A more accurate estimate of nitroso (-NO) should be obtained, and the following should be considered:

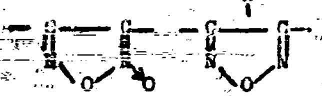
1. Of interest for explosives

a) azide $-N_3$

b) 1,2,3-triazole and 1,2,4-triazole

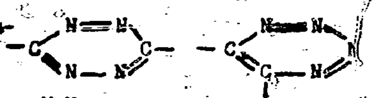


c) furoxan and furazan



d) triazene, pentazdiene, and other linear nitrogen chains -N=N-N- -N=N-N-N=N- etc.

e) 1,2,4,5-tetrazine and 1,2,3,4-tetrazine

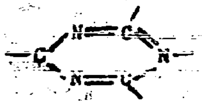


f) azine =N-N=

g) hydrazone =N-N-

h) imide -C(=O)-N-C(=O)-

i) s-triazine



j) imine or anil =N-

k) hydroxylamine -N-OH

l) nitrite -ONO

m) perchlorate ester $-OClO_4$

2. Of general interest

n) thiol -SH

o) sulfide -S-

p) disulfide -S-S-

q) sulfonic acid $-SO_3H$

r) chloro -Cl

s) bromo -Br

t) iodo -I

u) isocyanate -NCO

v) peroxide -O-O-

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E. Rules and Procedure for Calculating Heat of Combustion with Examples

The present system described in this report is based on the assumption, adequately upheld by experimental evidence, that the molar heat of combustion of any organic homologous series bears a straight line relation, within an acceptable limit of error, to the number of atoms of oxygen lacking in the molecule which are required to burn the compounds to CO_2, H_2O, N_2, HX, and SO_2. A quick estimation of this number, called the molar oxygen balance, for the compound, $C_mH_nN_pO_qX_rS_t$ can be made by the equation: Oxygen balance $= 2(n+t) + \frac{(n-r)}{2} - q$.

Linear equations for a large number of functional types have been obtained by the method of least squares. The slope and intercept values for these equations related to the paraffin equation as a basis are given in Table 60, and the heat of combustion data used for the estimation are given in Tables 61 through 138. At present calculations are limited to compounds containing the groupings given in Table 60. The data were taken from many sources, and the only correction applied to the original data, aside from correcting obvious errors, was to convert the results reported to a basis of constant pressure, where necessary.

Fundamental Rule

The heat of combustion of a compound is computed from the oxygen balance of the compound on a molar basis and the equation derived from the summation of the slope and intercept factors for each structural feature, including paraffin as one of the features in every case. Thus $Q_c^p = \sum a_i' + x\sum b_i'$

in which a_i' = intercept coefficient for each functional type.

b_i' = slope coefficient for each functional type.

x = atoms of external oxygen required for combustion.

The system, in effect, calculates and applies the equation for the homologous series which has the same functional groups as the compound in question.

In Table 59 a few examples of the use of the equation illustrate the additional rules which have been followed in the derivation of the coefficients given in Table 60. Examples 5 and 6 illustrate larger and more complicated molecules which can be handled easily by the present system.

Rule 1.

The values for normal paraffins ($a = 5.7$ and $b = 52.08$) are always part of the equation, and it is considered that never more than one of this feature is ever present.

Rule 2.

If a chain is branched, or there is more than one alkyl substitutent attached to a cyclic structure the values for branched paraffin are added to the equation, but never more than one of these features is ever considered to be present. Thus benzene and toluene are not branched, but xylene, i-propylbenzene, and hexamethylolcyclohexane each has one branched paraffin feature. (See example 1, Table 59).

Rule 3.

If more than one functional group of the same type is present, the intercept term (a') is multiplied by the number of such groups, but the slope term is the same as for a single such group. The only exceptions to this rule are the normal paraffin and branched paraffin features. This rule is illustrated in example 1, Table 59, with six nitrate groups.

Rule 4.

When there is a choice between two possible groups, the values for the group which appears later in the table of coefficient (Table 60) are taken. In example 2, Table 59, although a formamide can be considered as both an aldehyde and an amide, only the amide values are taken in order to avoid duplicating groups. Incidentally, the amide value is about the same as the sum of an aldehyde and an amine, which is the alternate choice that could be made in the example shown. Exceptions to this rule of duplication are the urea type of group (-N-C(=O)-N-) and the biuret type of group (-N-C(=O)-N-C(=O)-N-) both of which are considered to be diamides. In addition the biuret group has an amine group as one of the components of the equation. It is hoped that such questions of duplication, which arise only with nitrogen containing compounds, can be resolved or avoided by use of bond contributions rather than group contributions. This may be done at a later date.

Rule 5.

Where a choice of coefficients is possible, depending on physical state, the ones taken are those corresponding to the physical state of the compound under consideration. Some exceptions to this rule are made in Table 60 when one set of coefficients is less reliable than the other, such as acid anhydride (solid is preferred to liquid), ester, nitrile, and secondary amine for which liquid is preferred to solid. Benzene (solid) and primary amine (solid) are reserved for hydrocarbons and aromatic amines, respectively. Derivation of coefficients for the liquid and solid phases have been based on normal paraffin (liquid) in all cases, and for the gas phase have been based on normal paraffin (gas) in all cases.

Rule 6.

With salts of organic bases and inorganic acids, and with hydrates, an additional step is required. The heat of combustion of the component base is calculated independently, by the general scheme, then added to the heat of combustion of the inorganic acid along with the value for each salt link, to give the heat of combustion of the salt. This is illustrated in example 3, Table 59. For inorganic components, such as nitric acid, the heat of combustion is computed from the heat of formation obtained from other sources. A similar procedure is adapted for salts of organic acids and inorganic bases. For organic salts, with carbon-carbon bonds, the ordinary rules for calculation can be followed. (See example 4, Table 59).

Rule 7.

For certain nitrogen containing groups there must be added to the contribution given in Table 60 additional values for amine or hydrazine when a carbon-nitrogen or nitrogen-nitrogen bond has been formed by substitution. Such is the case for amide, hydrazine, hydrazide, azo, azoxy, guanidine, tetrazole, nitramine, nitramide, nitrosamine, and nitrosamide. Thus a primary nitramine is considered to have both a nitramine and a primary amine contribution, and an N-substituted nitramide also has a primary amine contribution. To calculate an organic azo compound of the type Ar-N=N-Ar two primary amine contributions besides the azo, aromatic and paraffin features must be included. As in examples 2 and 3, Table 59, an N-substituted amide or guanidine should be considered to possess appropriate amine features in addition to the amide and guanidine contributions.

Rule 8.

For compounds which have functional groups not covered specifically in Table 60 approximations sometimes can be made by using values for a closely related group. This rule may be applied particularly to the physical state aspect. Little error will be introduced in most organic compounds if the value for the liquid state is used for solids, and vice versa. (See Rule 5). Compounds containing other structural features cannot be estimated at this time.

The data for homologous series of compounds in the same physical state were used to estimate the best straight line. In several instances enough data were available to give equations for more than one physical state for compounds containing a given functional group. The differences between the equations, then, would be the heat of fusion or heat of vaporization for the homofunctional types. The differences due to heat of fusion for organic compounds are small, particularly for the less polar types, but it is felt that account should be taken of this factor where it is possible to do so, reducing at least one source of error. However, the error of using liquid data for solid compounds is small.

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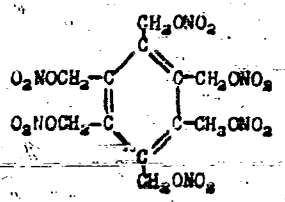
TABLE 59

Illustration of Heat of Combustion Calculation

$$Q_C^p = \Sigma a' + x \Sigma b'$$

1. Hexamethylolbenzene hexanitrate (183)



Q_C^p (obs) = 1396.1 kcal/mole Ref. 71

$C_{12}H_{12}N_6O_{18}(s) + 6\ O_2 \rightarrow 12\ CO_2 + 6\ H_2O + 3\ N_2$

x = 12

	a' (intercept)	b' (slope)	
1 normal paraffin (liq)	+ 5.7	+52.08	(Rule 1)
1 branched paraffin (liq)	- 3.7	+ 0.09	(Rule 2)
1 benzene (liq)	-10.1	+ 0.07	(Rule 5)
6 ONO_2 (s) 6 x 128.4 =	+770.4	+ 0.53	(Rule 3)

Q_C^p = 762.3 + (12.0) (52.77) = 1395.7 kcal/mole

2. Dimethylformamide $HC(=O)N(CH_3)_2$

Q_C^p (obs) not found

$C_3H_7NO(liq) + 4.25\ O_2 \rightarrow 3\ CO_2 + 3.5\ H_2O + 0.5\ N_2$

x = 8.5

	a' (intercept)	b' (slope)	
1 normal paraffin (liq)	+ 5.7	+52.08	(Rule 1)
1 amide (liq)	- 5.6	+ 0.47	(Rule 4)
1 secondary amine (liq)	+18.3	- 0.12	(Rule 7)

Q_C^p (calc) = 18.4 + (52.43) (8.5) = 464.1 kcal/mole

3. Diaminoguanidine nitrate $NH_2NHC(=NH)NHNH_2 \cdot HNO_3$

Q_C^p (obs) = 329.8 kcal/mole (59)

$CH_8N_6O_3(s) + 1.5\ O_2 \rightarrow CO_2 + 4\ H_2O + 3\ N_2$

x = 5.5 (for diaminoguanidine) (Rule 6)

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TABLE 59 (cont'd)

	a' (intercept)	b' (slope)	
1 normal paraffin (liq)	5.7	52.08	(Rule 1)
1 guanidine (s)	0.7	+ 0.46	(Rule 7)
2 hydrazine bonds (s)	65.0	- 0.10	(Rule 7)

Q_C^P (calc) = 71.4 + (51.52) (5.5) = 354.8 kcal/mole for diaminoguanidine

1 salt link	-14.0	(Rule 6)
1 HNO_3	- 7.2	

Q_C^P (calc) = 354.8 - 14.0 - 7.2 = 333.6 kcal/mole for diaminoguanidine nitrate

4. Carbohydrazide hydrogen oxalate $NH_2NHC(=O)NHNH_2 \cdot (COOH)_2$

x = 5.0 (for entire molecule) (Rule 6)

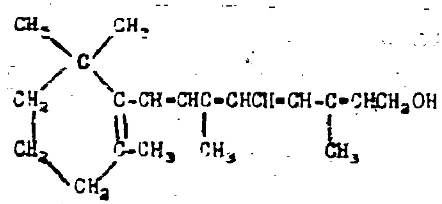
Q_C^P (obs) = 314.6 kcal/mole Ref. 96

$C_3H_8N_4O_5(s) + 2.5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O + 2\ N_2$

	a' (intercept)	b' (slope)	
1 normal paraffin (liq)	+ 5.7	+52.08	(Rule 1)
2 hydrazide (s) (2 x 28.7) =	+57.4	- 0.09	(Rule 3,7)
2 acid (s) (2 x -3.8) =	- 7.6	- 0.01	(Rule 3,5)
1 salt	-14.0	-	(Rule 6)

Q_C^P = 41.5 + (51.98) (5) = 304.0 kcal/mole

5. Vitamin A (Carotene)



$C_{20}H_{30}O(s) + 27\ O_2 \rightarrow 20\ CO_2 + 15\ H_2O$

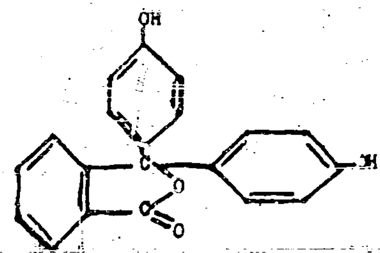
x = 54

	a' (intercept)	b' (slope)	
1 normal paraffin (liq)	5.7	52.08	(Rule 1)
1 branched paraffin (liq)	- 3.7	+ 0.09	(Rule 2)
1 cyclohexane (liq)	- 7.4	0.00	(General)
5 normal olefin (liq) 5 x (14.2) =	+71.0	- 0.01	(Rule 3)
1 primary alcohol (liq)	+ 9.2	- 0.05	(Rule 5)

Q_C^P = 74.8 + (52.11) (54) = 2888.7 kcal/mole

TABLE 59 (cont'd)

6. Phenolphthalein



$C_{20}H_{14}O_4(s) + 21.5\ O_2 \longrightarrow 20\ CO_2 + 7\ H_2O$

x = 43

	a' (intercept)	b' (slope)	
1 normal paraffin (liq)	5.7	52.08	(Rule 1)
1 branched paraffin (liq)	- 3.7	+ 0.09	(Rule 2)
3 benzenes (liq)	-10.1	+ 0.07	(Rules 5 and 3)
2 aromatic hydroxyl (s)	+ 7.0	- 0.29	(Rule 3)
1 ester (liq)	+16.1	- 0.42	(Rule 5)

$Q_C^p = 15.0 + (51.53)(43) = 2230.8$ kcal/mole

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TABLE 60

COEFFICIENTS OF EQUATIONS FOR HEAT OF COMBUSTION

$$Q_C^p = \sum a' + x\sum b'$$

Normal paraffin (a = 5.7, b = 52.08

Normal paraffin (g   a = 5.5, b = 52.48

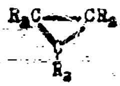
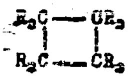
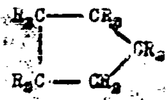
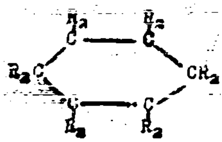
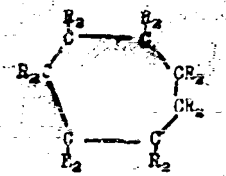
Functional Type	a' (intercept)	b' (slope)	
(R=aliphatic chain or hydrogen			
Paraffin branched (liq)	- 3.7	+0.09	
Cyclopropane (liq)	+16.2	-0.13	
Cyclobutane (liq)	+10.3	+0.11	
Cyclopentane (liq)	- 1.7	0.00	
Cyclohexane (liq)	- 7.4	0.00	
Cycloheptane (liq)	+17.1	-0.99	
Olefin			$R_2C{=}CR_2$
normal (liq)	+14.2	-0.01	
normal (gas)	+14.2[a]	0.00[a]	
Acetylene			$RC{\equiv}CR$
normal (liq)	+37.3	0.00	

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TABLE 60 (cont'd)

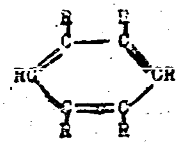
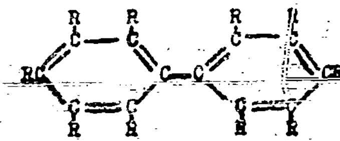
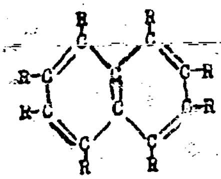
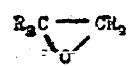
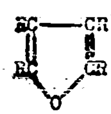
Functional Type	a' (intercept)	b' (slope)	
Benzene (liq)	-10.1	+0.07	
(gas)	- 7.0[a]	0.00[a]	
(solid)	-16.5[b]	+0.45[b]	
Biphenyl (liq)	-31.3	+0.37	
Naphthalene (solid)	- 6.1	-0.59	
Alcohol			
primary (liq)	+ 9.2	-0.05	RCH_2OH
primary (gas)	+18.3[a]	-0.24[a]	
secondary (liq)	+ 4.5	-0.44	$(R_3C)_2CHOH$
tertiary (liq)	+ 8.6	-0.95	$(R_3C)_3COH$
mixed (liq)	+10.3	-0.63	
mixed (solid)	+ 3.8	+1.27	
Aromatic hydroxyl (solid)	+ 7.0	-0.29	
Ether (liq)	+15.5	+0.02	R_3COCR_3
(gas)	+28.1	-0.05[a]	
Oxirane (ethylene oxide) (liq)	+41.2	-1.05	
Furan (liq)	+35.5	-1.17	
Aldehyde (liq)	+11.5	-0.09	RC(=O)H
(gas)	+20.9	-0.68	
Ketone (liq)	+ 5.5	-0.19	RC(=O)R

TABLE 60 (cont'd)

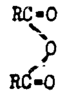
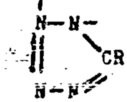
Functional Type	a' (intercept)	b' (slope)	
Acid (liq)	- 4.7	+0.07	RCOOH
(solid)[c]	- 3.8	-0.01	
Acid anhydride (liq)[d]	+ 9.2	-0.03	
(solid)	+ 2.4	-0.01	
Ester (liq)	+16.1	-0.40	RC(=O)OR
(solid)[e]	+16.1	-0.62	
Nitrile (liq)	+ 9.3	-0.01	RC≡N
(solid)[e]	+ 8.9	+0.29	
Carbylamine (Isonitrile) (liq)	+26.5	+0.57	RNC
Amine			
primary (liq)	+17.7	-0.81	R_3CNH_2
primary (gas)	+18.0[a]	-0.49[a]	
primary (solid)	+ 4.3[f]	-0.08[f]	
secondary (liq)	+18.3	-0.12	$(R_3C)_2NH$
secondary (solid)	-44.9[g]	+1.82[g]	
tertiary (liq)	+20.5	+0.08	$(R_3C)_3N$
Amide (liq)[h]	- 6.5	+0.57	RC(=O)N-
(solid)[h]	- 6.0	+0.16	
Hydrazine (solid)[h]	+32.5	-0.10	—N—N—
Hydrazide (solid)[h]	+30.2	-0.15	RC(=O)N—N—
Azo (solid)[h]	+35.4	+0.11	—N=N—
Azoxy (solid)[h]	+32.5	+1.44	—N=N— (↓O)
Guanidine (solid)[h]	+ 0.7	-0.46	—N—C(=NH)N—
Tetrazole (solid)[h]	+48.7	+0.32	
Oxime (solid)	+45.3	-0.12	$R_2C=NOH$
Nitro			
aliphatic (liq)	+38.4	-0.38	R_3CNO_2
aliphatic (solid)	+92.8	-0.65	
aromatic (liq)	+97.9	-0.39	
aromatic (solid)	+92.2	-0.40	

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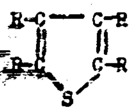
TABLE 60 (cont'd)

Functional Type	a' (intercept)	b' (slope)	
Gem trinitro (liq)	+292.5	+0.29	$RC(NO_2)_3$
(solid)	+288.2	-0.32	
Nitrate (liq)	+129.4	+0.23	R_3CONO_2
(solid)	+128.4	+0.53	
Nitramine (solid)[h]	+ 95.3	+0.81	$-\underset{\vert}{N}NO_2$
Nitramide (solid)[h]	+103.6	+0.10	$R\underset{O}{\underset{\Vert}{C}}NNO_2$
Fluorine (liq)	+ 10.9	+0.61	R_3CF
(solid)	+ 14.2	-0.19	
Gem trifluoro (liq)	+ 36.1	-0.44	RCF_3
Nitrosamine (solid)	+ 56.0	+1.05	$-\underset{\vert}{N}NO$
(liq)			
Thiophene (solid)	+ 21.5	+0.98	
(liq)			
Nitroso (solid)	+ 20.9	+1.93	R_3CNO
Salt formation	- 16.1	-	
Hydrate formation	+ 4.5	-	

a) Based on normal paraffin (gas) value.
b) For hydrocarbons only.
c) From dibasic acids.
d) Based on small amount of data and not as reliable as value for solid.
e) Based on limited amount of data and less reliable than value for liquid.
f) From aromatic amines only.
g) Of questionable accuracy. Based on limited amount of data.
h) For substituents on the nitrogen atom(s), add appropriate bond-group values. Add primary amine values for one substituent on nitrogen, secondary amine values for two substituents on the same nitrogen.

F. Tables of Data

1. Scope

An attempt has been made to obtain from the literature, open and classified, all heats of combustion which have been published between 1929, when the bibliography by Kharasch (55) appeared, and 1951. Much of the material found appears in Tables 61 through 130, the omissions being compounds which do not fall into any homologous series reported there. With some exceptions, notably in the nitro and nitrate functions, heats of combustion before 1929 which have been used are the ones as given by Kharasch (55), but all of the heats reported by Kharasch have not been used or reproduced in the present treatise. However, all known heats of combustion of organic compounds containing the nitro or the nitroso group attached to carbon, oxygen or nitrogen have been included in this report even though there is duplication of compounds.

The primary source of the open literature data was Chemical Abstracts, for the years 1929-1951. In many cases the original publication cited by Chem. Abstr. was consulted for evaluation of the author's work, but this was not a universal rule. Classified literature covered included OSRD reports of Division 8, SPIA/M3 reports, Picatinny Arsenal Technical Reports, various current reports of Navy installations and contractors, and original work done for Arthur D. Little, Inc. by its subcontractors.

2. Method of Obtaining Least Squares Equations

The equation, $Q_c^p = a + bx$, was obtained for the paraffin hydrocarbons from the formulas:

$$b = \frac{n\sum xy - \sum x \sum y}{n\sum x^2 - (\sum x)^2}$$

$$a = \frac{\sum y - b\sum x}{n}$$

in which x = molar oxygen balance
y = heat of combustion at constant pressure
n = number of items.

The equations for the remaining homologous series were obtained by the same formulas from what might be called "reduced data", i.e. the values of Q_c^p remaining after subtracting 5.7 and the contribution of functional groups in the molecule other than the one being processed. To obtain x' and y' for least squares computation the reduced value for Q_c^p and the molar oxygen balance of the compound were then each divided by the number of like functional groups which were being calculated. Thus the equations were obtained literally for functional groups of a single type regardless of the presence of other groups in the compounds. This approach allowed the use of a larger body of available data than possible if only the data for pure, homofunctional types had to be used.

3. Arrangement of Heat of Combustion Data

Tables 61-138 contain the data of interest to this project. They have been arranged in general order of increasing complexity of functional type, although the equations were not all determined in the order in which they appear in the tables. The columns are self-explanatory. The ADL numbers are those assigned in Part I of this report (69) and as extended in Table 139. Many of the compounds have been renamed here to conform to accepted usage which avoids ambiguity. The numbers originally assigned in Part I (69), however, have not been changed.

Each of the Tables 61-138 shows the equation for the homologous series represented and the summation figures for its derivation. All combustion data above it were used for its calculation. The combustion data below the equation were not used but have been included for completeness, or because the data are pertinent to the field of explosives. An occasional entry made below the equation was found too late to include in the calculations.

The heat of hydration was determined as an average from pairs of data for hydrates and the anhydrous compound (Table 134). The heat of salt formation was obtained as the difference between the heat of formation (or combustion) of the salt and the sum of the heats of formation (or combustion) of the basic and acidic components of the salt. (Table 135).

G. Historical

Methods of calculating heats of formation and of combustion for organic compounds have been used for many years. They can be divided into four general types:

1. Methods of summation, using bond, resonance, and group energies. These generally have a sound basis in theory and have been well-developed for fairly wide application. The energy values are obtained from considerations of observed thermochemical data.

2. Methods of summation, using a base value to which are added corrections for substituent functional groups. These are generally empirical and based on observed data.

3. Methods based on linear equations obtained from relationships between heat value and some intrinsic feature of a series of homologous compounds, such as number of carbon atoms in the molecule or parachor. These are empirical methods using observed data but of limited applicability.

4. Methods involving effects observed upon substituting one group for another. These have been widely used but are extremely limited or completely unsuitable for prediction of thermochemical properties of new or unknown structures.

1. Methods of Summation of Bond Energies

The method which has probably received the greatest popular attention is that based on the additivity of bond energies as outlined by Pauling (89) for heats of formation, and expanded and extended by Wheland (20) and Klages (59) to heats of combustion. The bond values given by Pauling (89) were determined from thermochemical considerations of small molecules as given by Bichowsky and Rossini (16)

Wheland (20) in explaining the theory of resonance and comparing values for different resonant structures, converted Pauling's bond energies of formation to values which could be used to estimate heat of combustion. Klages (59) later improved the accuracy and added to the values of Wheland, enlarging the scope and applicability of this system.

Springall and Roberts (130) obtained a set of bond, resonance, and group energies for heats of formation especially suitable for explosive compounds containing carbon, hydrogen, nitrogen, and oxygen. Pauling's bond energies were taken as a basis, and group energies were determined from known heats of formation for a great many explosive compounds.

In the present continuing investigation it was felt that heat of combustion was a more valuable and accessible function than heat of formation. Part II of this report by Arthur D. Little, Inc., (70) presented bond and group energies for calculating heats of combustion which were determined for the special field of explosives along the lines of Springall and Roberts (130).

Anderson, Beyer, and Watson (3) reported a system of group contributions for calculating heats of formation, entropies, and heat capacities of organic compounds. The development of their system was based on theoretical consideration and "heats of atomization".

All of these methods, except that of Arthur D. Little, Inc., as described in Part II (70), produce results for compounds in the gaseous state and appropriate corrections must be assumed to convert them to values for the standard state of the compounds of which the great majority are solid or liquid. All the preceding systems of bond and group energies become exceedingly difficult to apply to complex groups and heterocyclic structures.

A good discussion of the early methods proposed for calculating heats of formation in the gaseous state from bond energies is given by Rossini (114). Major contributions to these methods, besides those described above (3, 69, 130), have been made by Anderson and Gilbert (5), Coates and Sutton (25), and Cole and Gilbert (26). Resonance energies of ring structures were introduced into the system of bond energies by Wheland (20), and additional values have been obtained by Willis (2, 151) and by workers at the Naval Ordnance Test Station (77).

Efforts to improve the accuracy of calculated heats of formation have been made by Laidler (62, 63) who used a system similar to Pauling's and Wheland's but based it on bond strengths and "heats of atomization." Laidler's method suffers from being too complicated for use with polyfunctional compounds and the accuracy claimed for functional types other than hydrocarbons is misleading, since values given are based on a limited amount of unconfirmed data in the early literature. Others have attempted to apply group contribution methods to heat of formation taking into account neighboring effects (37, 97, 127). These are all rather theoretical treatments, Platt (97) limiting his calculations to paraffin hydrocarbons, and Souders (127) to hydrocarbon vapors. Franklin (37) attempted to include many of the more common functional groups but used very limited data to obtain his figures. His suggestions are also very difficult to apply to complicated configurations.

Stern and Klebs (131, 132), from a study of heats of combustion of pyrroles, determined thermochemical characteristics for a large number of common functional groups attached to the heterocyclic nucleus.

Of more theoretical interest are the investigations of bond strengths by Cottrell and Sutton (30), Walsh (150), and Skinner and Springall (126). Cotrell (28) also calculated binding energies of hydrocarbons and resonance energies of simpler aromatic hydrocarbons. Roberts and Skinner (112) derived heats of formation of a number of alkyl radicals and resonance energies from thermal and other data.

Methods for calculating heats of formation from structural groups and molecular formulas, employing standard equations, have been suggested (19, 22, 105, 106), and heats of combustion have been calculated by similar methods (20, 21). All of these results were limited to gaseous hydrocarbons. Another author (42) adopted 8, the lowest even calculated value for bond energies published, as the unit of the chemical bond and calculated heats of formation from energies of all other bonds grouped as multiples of this unit.

2. Methods of Summation using a Base Value plus Group Corrections

One of the best and most thoroughly described methods for calculating heats of combustion from the structure of an organic compound is that described by Kharasch (55). Kharasch and Sher (56) have given the background and basis for his method of calculation which depends on adding the number of electrons in a molecule multiplied by the combustion value of each electron, to the corrections for structural and functional features. Aerojet Corp. (1) has extended the system to include primary phosphoric types (69) of compounds. The method is more empirical and less theoretical than those described previously in this report, and in general gives good agreement with observed values. The physical state is liquid which involves fewer corrections and assumptions to compute values for most compounds. It is not adapted to heterocyclic compounds, however, and does not always work well with the more complicated functional groups.

3. Methods Based on Linear Equations

The Kharasch theory of molar summation has been converted to a weight basis (52). Results are expressed in a unique series of graphs for a single functional type, with heat of combustion plotted against percent carbon in the compounds. Heats of combustion and formation are tabulated in the form of general equations for the different classes of compounds. The method has not been used, however, with poly- and heterofunctional molecules.

One author (68) has attempted to establish a relationship between atomic number, effective nuclear charge, and heat of combustion for compounds containing C, H, and O, and another (43) has proposed a relationship between heats of combustion and composition of organic compounds by use of a single simple formula. It is not easy to see how these systems have general applicability and validity.

The values of the parachor and the heats of combustion or formation of organic compounds have been correlated by a straight line relationship (95). The values of the slope and intercept are different for various homologous series and classes of compounds, but it is claimed they can be determined easily if the values of parachor and combustion are known for one of the representatives of a homologous series. Slope and intercept values for nine homologous series are given. Satisfactory agreement between experimental and calculated values is illustrated with saturated alcohols.

Numerous articles have been published giving empirical methods for calculating heats of combustion from observed data. Heat of combustion of successive members of homologous series have been obtained by Verkade and co-workers from which was calculated the heat of combustion for the methylene ($-CH_2-$) group. Thus the straight chain dicarboxylic acids (143) and their dimethyl esters (146), the homologous normal primary aliphatic alcohols (144), and monoalkyl-substituted malonic acids (145) have been studied. Banse and Parks (11) did much the same thing for paraffin hydrocarbons. Schjanberg (123) calculated the energy of cleavage of the C-Cl link in a series of aliphatic monocarboxylic acids and their esters, relating it to the change in position of the halogen.

Rossini and co-workers applied similar techniques. Relating the number of carbon atoms in a series of normal aliphatic primary alcohols to their heats of combustion, he found that a straight line would express the heat of combustion for alcohols longer than pentanol (113). The equation given is

$$Q_c = 21.60 + 157.00\ n \quad \text{(gaseous state)}$$
$$= 12.00 + 157.00\ n \quad \text{(liquid state)}$$

in which n, the number of carbon atoms, must be greater than 5. Similar equations applicable to the estimation of heats of combustion of paraffin hydrocarbons were calculated (103), giving

$$Q_c = 57.909 + 157.443\ n \quad \text{(gaseous state)}$$
$$= 57.430 + 156.263\ n \quad \text{(liquid state)}$$

in which n, again, is the number of carbon atoms, and is greater than 5. An equation obtained for alkylbenzenes (100) is:

$$Q_c = -158.990 + 157.443\ n \quad \text{(gaseous state)}$$

in which n is the number of carbon atoms, and is greater than 9.

A straight line for approximating the heat of combustion of gasolines from the percent of hydrogen has been proposed recently (53a).

Lantié (65) gave straight line equations for calculating heats of combustion of eleven homologous series of compounds with commonly encountered functional groups. Agreement with observation was good, but no attempt was made to expand the system to poly- or hetero-functional compounds. For calculating heats of formation he gave a treatment similar to Sugden's parachor.

Holcomb and co-workers found a straight line relationship between oxygen balance and heat of combustion (on a weight basis) for nitroalkanes (44) and later for nitroalcohols (31a). Earlier a straight line relationship was reported between the weight heat of combustion and oxygen balance of explosives, in which different lines were found for different types (23). The value of substituting an aromatic alkyl ether for an aromatic hydroxyl group in explosives was also determined.

4. Methods Based on Group Substitutions

One of the most common methods of predicting heats of formation and combustion is based on the effects observed upon substituting one group for another. Although frequent publications have been made comparing classes of compounds differing only in a single functional group, prediction of heat values is limited to such comparisons, and has not generally been extended to prediction from additive structural features, or to unknown compounds. Thus Swietoslawski (Svyentoslavskii) (135) obtained thermochemical characteristics of many groupings including -N=O, -N-N-, -N=N-, and $-NO_2$. By a similar technique the effect of a nitro group on heat of combustion has been found from a study of aromatic nitro derivatives (137) and there has been calculated the heats of combustion of certain groups such as carbonyl, hydroxyl, olefin, etc. (12). A series of furans and benzenes has been compared (84). A study of furazan and furoxan compounds (80) showed a relation similar to the azo and azoxy derivatives according to LeMoult (67). The contribution of the oxime group has been calculated (81) and energy changes in the formation of chelate rings have been measured (17). Badoche has correlated the effects on heat of combustion of introducing nitro groups into the benzene ring (8), of introducing hydroxyl and methyl groups into the benzene ring (9), and of introducing hydroxyl groups into the benzene ring (10) already containing nitro groups. Matignon investigated the difference between a nitroso substituted on carbon and on nitrogen (75) and applied the information gained from the effect of adding a methyl group to a nitrogen atom in cyclic ureas to deduce and establish formulas of constitution (74). The effect of introducing successive nitro groups into aromatic rings and the relationship of the heat of formation to the number of nitro groups present has been studied (110).

H. References

1. Aerojet Engineering Corp., Report No. 417 A, Contract N7onr-462 by Gold and Carlston (23 December 1949), pp. 31-36. CONFIDENTIAL.

2. A. Albert and J. B. Willis, Nature, 157, 341 (1946); C.A., 40, 3311 (1946). "Resonance energies of acridine and phenazine".

3. J. W. Anderson, G. H. Beyer, and K. M. Watson, Nat. Petroleum News, 36, 476 (1944). "Thermodynamic properties of organic compounds - Estimation from group concentrations". Also see O. A. Hougen and K. M. Watson, "Chemical process principles", Part II, John Wiley, New York (1947) pp. 758-765.

4. C. Anderson, L. G. Cole, and E. C. Gilbert, J. Am. Chem. Soc., 72, 1263-1264 (1950). "The heats of combustion of some isomeric nitrostilbenes and their isomerization energies".

5. C. M. Anderson and E. C. Gilbert, J. Am. Chem. Soc., 64, 2369 (1942). "The apparent energy of the N-N bond as calculated from heats of combustion".

6. Army-Navy Solid Propellant Group, Bulletin of 4th Meeting. (19-20 April 1948) and Addendum. CONFIDENTIAL

7. M. Badoche, Bull. soc. chim. [5], 4, 549-558 (1937); C.A., 31, 4196 (1937). "Determination of heats of combustion of several nitro derivatives of naphthalene".

8. M. Badoche, Bull. soc. chim., 6, 570-579 (1939); C.A., 33, 5736 (1939). "Determination of heats of combustion of nitro derivatives of the benzene series".

9. M. Badoche, Bull. soc. chim., 8, 212-220 (1941). C.A., 36, 1840 (1942). "Heats of combustion of phenol, m-cresol, and of their ethers".

10. M. Badoche, Bull. soc. chim., 9, 86-95 (1942); Chem. Zentr., 1942, II, 2013; C.A., 38, 2558 (1944). "The heat of combustion of nitrated phenol derivatives".

11. H. Banse and G. S. Parks, J. Am. Chem. Soc., 55, 3223 (1933) "Thermal data on organic compounds XII. The heats of combustion of nine hydrocarbons".

12. M. F. Barker, J. Phys. Chem., 29, 1345-1363 (1925); C.A., 20, 326 (1926). "Calorific value and constitution".

13. M. Beckers, Bull. soc. chim. Belg., 40, 518-610 (1931); C.A., 26, 2626 (1932). "Methods and equipment used at the Bureau of Physico-chemical Standards. V. VI. Heats of combustion".

14. Berthelot and Matignon, Compt. rend., 113, 246 (1891). "Heats of combustion and formation of nitrobenzenes".

15. Berthelot and Matignon, Ann. chim. et phys. (6), 30, 565 (1893). "Nitromethane and its homologues".

16. F. R. Bichowsky and F. D. Rossini, "Thermochemistry of the chemical substances", Reinhold, N. Y. (1936)

17. G. B. Bonino, R. Manzoni-Ansidei, and M. Rolla, Ricerca sci., 8, No. 5-6, 4 pp. (reprint) (1937); C.A., 32, 4846 (1938). "Experimental contributions to the problem of chelation. VI. Thermochemical investigations of acetylphenols and acetylresorcinols".

18. L. Brull, Gazz. chim. ital., 65, 19-28 (1935); C.A., 29, 3589 (1935). "Heats of combustion of some derivatives of biphenyl".

19. M. Brutzkus, Compt. rend., 204, 490-3 (1937); C.A., 31, 2579 (1937). "Intrinsic value of linkages C-C and C-H in hydrocarbons".

20. M. Brutzkus, Compt. rend., 204, 574-5 (1937); C.A., 31, 2916 (1937). "Thermochemistry of hydrocarbons".

21. M. Brutzkus, Compt. rend., 204, 959-61 (1937); C.A., 31, 3373 (1937). "Yields of combustion of hydrocarbons and energy values of the linkages of their atoms".

22. M. Brutzkus, Compt. rend., 204, 1802-4 (1937); C.A., 31, 5666 (1937). "Heat of formation of hydrocarbons".

23. E. Burlot, M. Thomas, and M. Badoche, Mem. poudres, 29, 226-282 (1939); C.A., 34, 1849 (1940). "Calorimetry of explosives".

24. Chemical Rubber Publishing Co., Cleveland, Ohio. "Handbook of Chemistry and Physics".

25. G. E. Coates and L. E. Sutton, J. Chem. Soc., 1948, 1187. "The heats of formation of the -N=N- and -C=N- bonds".

26. L. C. Cole and E. C. Gilbert, J. Am. Chem. Soc., 73, 5423-5427 (1951). "The heats of combustion of some nitrogen compounds and the apparent energy of the N-N bond".

27. J. Coops, D. Mulder, J. W. Dienske, and J. Smittenberg, Rec. trav. chim., 65, 128 (1946); C.A., 40, 3972 (1946). "The heats of combustion of a number of hydrocarbons (preliminary communication)". See also Rec. trav. chim., 66, 153-160 (1947); C.A., 41, 6460 (1947). "Heat of combustion. IV. Technique for the determination of heats of combustion of volatile liquids".

28. T. L. Cottrell. J. Chem. Soc., 1948, 1448-1453; C.A., 43, 2852 (1949). "Binding energies in hydrocarbons".

29. T. L. Cottrell and J. E. Gill, J. Chem. Soc., 1951, 1798-1800. "The preparation and heats of combustion of some amine nitrates".

30. T. L. Cottrell and L. E. Sutton, Quart. Rev., 2, 260-276 (1948); C.A., 43, 1230 (1949). "The interpretation of bond properties".

31. R. S. Crog and H. Hunt, J. Phys. Chem., 46, 1162-1163 (1942); C.A., 37, 1321 (1943). "Heats of combustion. II. Heats of combustion of ethyl methyl ketone and ethylene oxide".

31a R. M. Currie, C. O. Bennett, and D. E. Holcomb, Ind. Eng. Chem., 44, 329-331 (1952). "Heats of combustion of some nitro alcohols".

32. H. S. Davis and O. F. Wiedeman, Ind. Eng. Chem., 37, 483 (1945). "Physical properties of acrylonitrile".

33. M. Delepine, Bull. soc. chim., 15, 1199 (1896). "Hexamethylenetetramine and its nitroso derivatives: thermochemistry".

34. M. Delepine and M. Badoche, Compt. rend., 214, 777-81 (1942); C.A., 38, 5138 (1944). "The thermochemistry of CH_2O, $(CH_2)_6N_4$, and their derivatives".

35. P. dePauw, Z. ges. Schiess- u. Sprengstoffw., 32, 10-12, 36-37, 60-63 (1937); C.A., 31, 3696 (1937). "Heat of combustion of smokeless powder".

36. Fassler, "Dissertation", Dresde (1930).

37. J. L. Franklin, Ind. Eng. Chem., 41, 1070-1076 (1949). "Prediction of heat and free energies of organic compounds".

37a J. L. Franklin and H. E. Lumpkin, J. Am. Chem. Soc., 74, 1023-1026 (1952). "Some C-S, H-S and S-S bond strengths by the electron impact method".

38. Cl. Fromageot and E. Dammi, Bull soc. chim., 49, 929-936 (1931); C.A., 25, 5076 (1931). "The heat of combustion of methylglyoxal".

39. W. E. Garner and C. L. Abernethy, Proc. Roy. Soc. (London), 99A, 213-235 (1921); C.A., 15, 3748 (1921). "Heats of combustion and formation of nitro-compounds. Part I. Benzene, toluene, phenol and methylaniline series".

40. O. Glemser and V. Haussar, Z. Naturforsch., 3b, 159 (1948); C.A., 43, 3682 (1949). "Carbon monoxide compounds of the nonmetals. II. Properties of carbonyl cyanide".

41. W. Gliwitzky, Feuerschutz, 19, 80-82 (1939); C.A., 33, 8415 (1939). "Naphthalene dust and vapor explosions".

42. A. Gosselin, Bull. soc. chim., 12, 61-67 (1945); C.A., 40, 4267 (1946). "The unit of the chemical bond (energy)".

43. A. Harlin, IVA, 17, No. 1, 28 (1946); C.A., 40, 5525 (1946). "Elementary analysis and heat of combustion".

44. D. E. Holcomb and C. L. Dorsey, Jr., Ind. Eng. Chem., 41, 2788-2792 (1949). "Thermodynamic properties of nitroparaffins".

45. W. N. Hubbard, J. W. Knowlton, and H. M. Huffman, J. Am. Chem. Soc., 70, 3259 (1948). "The heat of combustion of 2,2'-bis-(4-hydroxy-phenyl)-propane".

46. W. Huckel, A. Gercke and A. Gross, Ber., 66B, 563 (1933); C.A., 27, 4811 (1933). "Cyclodecane".

47. H. M. Huffman, J. Am. Chem. Soc., 60, 1171-1177 (1938). "Thermal data. IX. The heats of combustion of hippuric and succinic acids and a proposal for the use of hippuric acid as a secondary standard in combustion calorimetry".

48. H. M. Huffman, J. Am. Chem. Soc., 62, 1009 (1940). "Thermal data. XII. The heats of combustion of urea and guanidine carbonate and their standard free energies of formation".

49. H. M. Huffman, E. L. Ellis, and S. W. Fox, J. Am. Chem. Soc., 58, 1728 (1936). "Thermal data. VI. The heats of combustion and free energies of seven organic compounds containing nitrogen".

50. A. M. Hughes, R. J. Corruccini, and E. C. Gilbert, J. Am. Chem. Soc., 61, 2639 (1939). "Studies on hydrazine: The heat of formation of hydrazine and of hydrazine hydrate".

51. H. Hunt and P. F. Stehlo, Purdue University, Private Communication.

52. E. Janecke, Z. Elektrochem., 40, 462-469 (1934); C.A., 28, 6364 (1934); cf C.A., 25, 3226 (1931). "The heats of combustion and formation of organic compounds in relation to their structure".

53. R. S. Jessup, J. Research Nat. Bur. Standards, 20, 589 (1938). "Heat of combustion of isoprene".

53a. W. H. Jones and C. E. Starr, Ind. Eng. Chem. Anal. Ed., 13, 287-290 (1941). "Determination of the heat of combustion of gasolines".

54. H. Kast. Chem. Zeit., 1925, 621 (As given by Burlot, Ref. 27).

55. M. S. Kharasch, Bur. Standards J. Research, 2, 359-430 (1929). "Heats of combustion of organic compounds".

55-9. E. Berner, Arch. Math. Naturvidenskab, 36, No. 6, 5-134 (1926); C.A., 21, 3814 (1927). "A contribution to the thermochemistry of organic compounds".

55-24. Berthelot and G. Andre, Ann. chim. et phys. (7), 17, 433 (1899). "New studies on the heats of formation and combustion of various nitrogen compounds and others".

55-25. Berthelot and Delepine, Compt. rend., 129, 920 (1899). "Lactic acid".

55-26. Berthelot and Delepine, Ann. chim. et phys. (7), 21, 289 (1900). "Heat of combustion of very volatile liquids".

55-34. Berthelot and Matignon, Compt. rend., 114, 1145 (1892). "Heats of combustion and formation of alcohol and formic and acetic acids".

55-37. Berthelot and Matignon, Ann. chim. et phys. (6), 30, 547 (1893).

55-41. Berthelot and R. P. Petit, Ann. chim. et phys. (6), 18, 107 (1889). "Heats of combustion and formation of nitriles".

55-44. Berthelot and Rivals, Ann. chim. et phys. (7), 7, 29 (1896). "New studies on thermochemical relations between aldehydes, alcohols, and acids".

55-51. P. Bruylants and A. Christiaen, Bull. soc. chim. Belg., 34, 144 (1925). "Thermochemistry of the butene nitriles".

55-52 Bureau of Standards, Cir. 11, 3d. ed., (1917). "The standardization of bomb calorimeters".

55-54. J. Coops and P. E. Verkade, Rec. trav. chim., 44, 983 (1925). "Calorimetric researches. IX. The heat of combustion of d- and meso-tartaric acids, racemic acid and a number of their derivatives".

55-58. M. Delepine, Compt. rend., 131, 684 (1900). "Acetals of monohydroxy alcohols".

55-60. M. Delepine, Compt. rend., 132, 777 (1901). "Heat of formation of acetals compared to that of isomeric compounds".

55-64. A. G. Emery and F. G. Benedict, Am. J. Physiol., 28, 301, (1911). "The heat of combustion of compounds of physiological importance".

55-65. P. A. Favre and J. T. Silbermann, Ann. chim. et phys. (3), 34, 357 (1852). "Researches on the quantities of heat released in chemical and molecular reactions".

55-66. Fischer and Wrede, Sitsber. kgl. preuss.Akad. Wiss., 1904, 687.

55-77. H. Guillemard, Ann. chim. et phys. (8), 14, 311 (1908). "Studies on the tautomerism of cyanogen derivatives".

55-78. J. Guinchant, Compt. rend., 121, 354 (1895). "Heat of combustion of some B-keto esters". Ibid., 122, 943 (1896). "Heat of combustion of cyano derivatives." All data collected and evaluated in Ann. chim., 10, 51 (1918). "Study of the acid function in methenic and methinic derivatives".

55-80. F. Henning, Z. physik. Chem., 97, 467 (1921). "Heats of combustion of benzoic acid, naphthalene, and cane sugar. A critical review".

55-93. Ph. Landrieu, Compt. rend., 140, 867 (1905). "Heat of formation of oximes".

55-97. P. Lemoult, Compt. rend., 143, 772 (1906). "Heat of combustion and formation of some cyclic nitrogen compounds".

55-98. P. Lemoult, Compt. rend., 143, 902 (1906). "Carbylamines and nitriles".

55-99. P. Lemoult, Ann. chim. et phys. (8), 10, 395 (1907). "Theorectical and experimental studies on the heats of combustion and formation of organic compounds. I. Primary, secondard, and tertiary amines".

55-100. P. Lemoult, Ann. chim. et phys. (8), 13, 562 (1908). "2. Hydrazine compounds".

55-101. P. Lemoult, Ann. chim. et phys. (8), 14, 184 (1908). "3. Azoxy compounds". Ibid., 14, 289 (1908). "4. Azo compounds".

55-102. P. Lemoult, Compt. rend., 148, 1602 (1909). "Comparison of nitriles and carbylamines".

55-110. W. Louguinine, Ann. chim. et phys. (5), 21, 139 (1880). "Heat released in the combustion of some isomeric alcohols of the fatty series as well as that of oenanthol".

55-113. W. Louguinine, Ann. chim. et phys. (5), 23, 384 (1881). "Heats of combustion of some alcohols of the allylic series and of aldehydes isomeric with them".

55-117. W. Louguinine, Compt. rend., 100, 63 (1885). "Heat of combustion of some substances of the fatty series".

55-118. W. Louguinine, Compt. rend., 101, 1061 (1885). "Heat of combustion of some substances of the fatty series". Ibid., 101, 1154 (1885). "Heat of combustion of some esters of organic acids".

55-119. W. Louguinine, Ann. chim. et phys. (6), 8, 128 (1886). "Measure of the heat of combustion of esters of some organic acids as a means of determining the heat of formation of these acids".

55-120. W. Louguinine, Ann. chim. et phys. (6), 11, 220 (1887). "Heat of combustion of fatty acids and of fats in which they occur".

55-127. W. Louguinine, Ann. chim. et phys. (6), 23, 179 (1891). "Study of the heat of combustion of some organic acids and anhydrides".

55-130. C. Matignon, Ann. chim. et phys. (6), 28, 70 (1893). "Ureides derived from acids with one and two carbon atoms". Ibid., 28, 289 (1893). "Polybasic ureides and uric acid. Ibid., 28, 498 (1893). "Some general results of the thermochemical study of ureides." These articles contain also the data reported by Matignon, Compt. rend., 110, 1267 (1890); 112, 128 (1891).

55-131. C. Matignon and Deligny, Compt. rend., 121, 422 (1895). "Nitro substitution".

55-138. C Moureu and E. Andre, Ann. chim. (9), 1, 113 (1914). "Thermochemistry of acetylenic compounds".

55-139. C. Moureu and J. Ch. Bougrand, Compt. rend., 170, 1025 (1920). "New studies on carbon subnitride. Action of halogens, halohydric acids, and alcohols".

55-141. C. Moureu, A. Boutaric, and C. Dufraisse, J. chim. phys., 18, 333 (1920). "Some physicochemical constants of acrolein".

55-142. J. A. Muller, Ann. chim. et phys. (8), 20, 116 (1910). "Heats of combustion and specific weights of methylamines".

55-147. P. Petit, Ann. chim. et phys. (6), 18, 145 (1889). "Researches on some nitrogen compounds of the aromatic series".

55-151. Reyer, Diss., Braunschweig (1923), quoted in Landolt-Bornstein Tabellen (1923).

55-153. T. W. Richards and H. S. Davis, J. Am. Chem. Soc., 42, 1599 (1920). "The heats of combustion of benzene, toluene, aliphatic alcohols, cyclohexanol, and other carbon compounds".

55-154. T. W. Richards and R. H. Jesse, J. Am. Chem. Soc., 32, 268 (1910). "The heats of combustion of the octanes and xylenes".

55-160. W. A. Roth, Rec. trav. chim., 45, 248 (1926). (Value by Lemoult corr. by Roth.) "A note on the work of Swietoslawski and Popow: 'Corrections of the thermochemical results of Lemoult'".

55-163. W. A. Roth, Unpub. work. Authority for these values in Landolt-Bornstein Tabellen. (1923).

55-172. W. A. Roth and Muller, Landolt-Bornstein Tabellen (1927).

55-175. W. A. Roth and G. J. Ostling, Ber., 46, 309 (1913). "Thermochemical studies in the alicyclic series."

55-179. J. Schmidlin, Ann. chim. et phys. (8), 7, 195 (1906). "Chemical and thermochemical studies on the constitution of rosaniline".

55-182. F. Stohmann, Z. physik. Chem., 6, 334-357 (1890). "Heats of combustion of organic compounds".

55-183. F. Stohmann, Z. physik. Chem., 10, 410-424 (1892). "Heats of combustion of organic compounds".

55-184. F. Stohmann and E. Haussmann, J. prakt. Chem. (2), 55, 263 (1897). "Calorimetric researches. 36. Calorific value of amide and anilide of the first member of the dibasic acid series". For details consult Ber. Verhandl. K. sachs. Ges. Wiss., 49, 1 (1897).

55-185. F. Stohmann and Kleber, J. prakt. Chem. (2), 43, 1 (1891).

55-187. F. Stohmann, Cl. Kleber and H. Langbein, J. prakt. Chem. (2), 40, 77 (1889). "Calorimetric researches. 17. Heat of combustion of benzene and other hydrocarbons of aromatic series".

55-189. F. Stohmann, Cl. Kleber and H. Langbein, J. prakt. Chem. (2), 40, 128 (1889). "Calorimetric researches. 18. Heat of combustion of carboxylic acids of the aromatic series".

55-190. F. Stohmann, Cl. Kleber and H. Langbein, J. prakt. Chem. (2), 40, 202 (1889). "Calorimetric researches. 19. Heat of combustion of acids of the oxalic acid series and of fumaric and maleic acids".

55-192. F. Stohmann, Cl. Kleber, H. Langbein, and P. Offenhauer, J. prakt. Chem. (2), 49, 99 (1894). "Calorimetric researches. 30. Heat of combustion of aliphatic acids". For details of the work consult Ber. Verhandl. K. sachs. Ges. Wiss., 45, 604 (1893).

55-193. F. Stohmann and H. Langbein, J. prakt. Chem. (2), 42, 361 (1890). "Calorimetric researches. 22. Fats and a fatty acid".

55-195. F. Stohmann and H. Langbein, J. prakt. Chem. (2), 45, 305 (1892). "Calorimetric researches. 26. Heat of combustion of carbohydrates, polyalcohols, and phenols".

55-201. F. Stohmann, P. Rodatz and H. Herzberg, J. prakt. Chem. (2), 33, 464-472 (1886). "Calorimetric researches. 7. Heat of combustion of phenol".

55-203. F. Stohmann, P. Rodatz and W. Herzberg, J. prakt. Chem. (2), 35, 22-42 (1887). "Calorimetric researches. 11. Heat of combustion of ethers of phenol".

55-204. F. Stohmann, J. prakt. Chem. (2), 35, 40, 136 (1887). "Calorimetric researches. 12. Heat of combustion of benzene homologs.

55-208. F. Stohmann and R. Schmidt, J. prakt. Chem. (2), 52, 59 (1895). "Calorimetric researches. 34. Heat of combustion of amides and anilides of monobasic acids". For details consult Ber. Verhandl. K. sachs. Ges. Wiss., 47, 1 (1895).

55-209. F. Stohmann and R. Schmidt, J. prakt. Chem. (2), 53, 345 (1896). "Calorimetric researches. 35. Heat of combustion of hippuric acid, its homologues, and of anisuric acid."

55-215. W. Swietoslawski, J. Am. Chem. Soc., 42, 1092 (1920). "The restatement and correction of the thermochemical data on organic compounds. 1. The data of P. W. Zubow".

55-216. W. Swietoslawski, J. chim. phys., 22, 583 (1925). "Remarks concerning the paper of W. Jaeger and H. V. Steinwehr titled: On the establishment of the heat of combustion of normal substances".

55-217. W. Swietoslawski, Private comm.

55-221. W. Swietoslawski and H. Starczewska, Bull. soc. chim. Belg. (4), 31, 654 (1922). "Heat of combustion of benzoic acid, cane sugar, and naphthalene".

55-223. J. Thomsen, Z. physik. Chem., 52, 343 (1905). "Numerical results of a systematic study of the heats of combustion and formation of liquid organic compounds".

55-225. A. Valeur, Ann. chim. et phys. (7), 21, 470 (1900). "Contribution to the thermochemical study of quinones. Study of the constitution of quinhydrones".

55-226. P. E. Verkade, Amst. Akad. Versl., 35, 496 (1926). Values by Verkade, van de Lee and Coops.

55-227. P. E. Verkade, Proefschr. Delft (1915).

55-238. E. Voisenet, Bull. soc. chim. Belg. (4), 17, 34 (1915). "Heats of formation of acrolein and of methacrolein".

55-239. H. v. Wartenberg, A. Muchlinski and G. Riedler, Z. angew. Chem., 37, 457 (1924). "Investigations of formaldehyde". See also H. v. Wartenberg and Lerner-Steinberg, Z. angew. Chem., 38, 591-592 (1925). "Heat of formation of formaldehyde".

55-243. P. W. Zubov, J. Russ. Phys.-Chem. Soc. (7), 28, 687 (1896).

55-245. P. W. Zubov and W. Swietoslawski, Bull. soc. chim. Belg., 37, 271 (1925). "Heat of combustion of three oxides".

56. M. S. Kharasch and B. Sher, J. Phys. Chem., 29, 625 (1925). "The electronic conception of valence and heats combustion of organic compounds".

57. O. M. Kibler and H. Hunt, J. Phys. and Colloid Chem., 53, 955-956 (1949); C.A., 43, 7318 (1949). "Heats of combustion. V. Five nitrogen-containing compounds".

58. J. Kielland, Ber., 71B, 220-226 (1938); C. A., 32, 2865 (1938). "Rapid colorimetric determination of potassium with hexanitrodiphenylamine (dipicrylamine) as well as some thermodynamic data concerning the amine and it potassium salt".

59. F. Klages, Chem. Ber., 82, 358-375 (1949) C.A., 44, 1323 (1950). "Improvement in the additive calculation of heats of combustion and the calculation of mesomerism energy from heats of combustion".

60. J. W. Knowlton and F. D. Rossini, J. Research Nat. Bur. Standards, 43, 113 (1949). "Heats of combustion and formation of cyclopropane".

61. P. N. Kogerman, Sitzber. Naturforsch. Ges. Univ. Tartu, 41, No. 3-4, 62pp. (1934); C.A., 29, 3297 (1935). "Addition reactions and polymerization of 2,3-dimethylbutadiene".

62. Catholic University of America, Contract NOrd 10260 Progress Report July 1 - December 31, 1949, by K. J. Laidler. " The estimation of heats of formation of organic compounds. Part I". RESTRICTED

63. Catholic University of America, Contract NOrd 10260, Final Report, 30 June 1950, by K. J. Laidler. "The estimation of heats of formation of organic compounds". RESTRICTED

64. P. Landrieu, F. Baylocq, and John R. Johnson, Bull. soc. chim., 45, 36-49 (1929); C.A., 23, 2967 (1929). "Thermochemical studies in the furan series".

65. R. Lautie, Bull. soc. chim. [5], 5, 1306-1321 (1938); C.A., 33, 1582 (1939). "Heats of formation and combustion".

66. A. Leman and G. Lepoutre, Compt. rend., 226, 1976-1978 (1948); C.A., 42, 8061 (1948). "Heats of combustion of naphthols".

67. P. LeMoult, Ann. chim. et phys. [8], 1, 496 (1903).

68. Lenhard, Z. Naturforsch., 4a, 257-261 (1949); C.A., 43, 8844 (1949). "Relationships between atomic number, effective nuclear charge, and heat of combustion".

69. Arthur D. Little, Inc., Contract W-19-020-ORD-6436 (2 January, 1947). "Study of pure explosive compounds. Part I. Correlation of organic structure with explosive properties from existing data". CONFIDENTIAL See also W. C. Lothrop and G. R. Handrick, Chem. Rev., 44, 419-445 (1949). "The relationship between performance and constitution of pure organic explosive compounds".

70. Arthur D. Little, Inc., Contract W-19-020-ORD-6436 (2 April, 1947). "Study of pure explosive compounds. Part II. Correlation of thermal quantities with explosive properties." CONFIDENTIAL

71. Arthur D. Little, Inc., Contract W-19-020-ORD-6436 and DA-19-020-ORD-12 (1 March, 1951). "Second report on synthesis and testing of high explosives". pp. 346-347. CONFIDENTIAL

72. W. C. Lothrop, G. R. Handrick and R. M. Hainer, J. Am. Chem. Soc., 73, 3581 (1951). "The structure and infrared absorption spectra of polynitrophenylmethylnitramines and polynitroanilines".

73. Mathieson Alkali Works, Inc., Lit. Report No. 76. "Uses and reactions of hydrazine". Revised April 1949.

74. C. Matignon, Ann. chim. et phys. (6), 28, 510 (1893). "General results of the thermochemical study of ureas".

75. C. Matignon and Deligny, Compt. rend., 125, 1103 (1897). "Difference between the nitroso substituted on carbon and on nitrogen".

76. M. Matui and T. Abe, Bull. Tokyo Univ. Eng., 8, 339-357 (1939); Chem. Zentr., 1941, I, 804; C.A., 37, 3 (1943). "Method of operation of an adiabatic calorimeter".

77. W. S. McEwan and M. W. Rigg, J. Am. Chem. Soc., 73, 4725-4727 (1951). "The heats of combustion of compounds containing the tetrazole ring".

78. C. B. Miles and H. Hunt, J. Phys. Chem., 45, 1346-1359 (1941); C.A., 36, 2469 (1942). "Heats of combustion. I. The heat of combustion of acetone".

79. A. J. Miller and H. Hunt, J. Phys. Chem., 49, 20-21 (1945); C.A., 39, 1352. "Heats of combustion. III. Heats of combustion of some polynitroparaffins".

80. M. Milone, Gazz. chim. ital., 61, 153-158 (1931); C.A., 25, 3624-3625 (1931). "Dioximes. LXXVI."

81. M. Milone and G. Venturello, Gazz. chim. ital., 66, 808-812 (1936); C.A., 31, 4646 (1937). "Dioximes. CIVIII".

82. H. Moureu and M. Dode, Bull. soc. chim. Belg. [5], 4, 637-647 (1937); C.A., 31, 4884 (1937). "Heats of formation of ethylene oxide, of ethanediol and some of their homologues".

82a. National Bureau of Standards, "Selected values of chemical thermodynamic properties. Series I." U. S. Dept. of Commerce, Washington, D. C. (30 June 1947).

83. Naval Ordnance Laboratory, Private Communication 4 October 1951 (Determined by National Bureau of Standards).

84. Naval Powder Factory, Quarterly Report 4 by F. C. Thames, 15 December 1948. CONFIDENTIAL.

85. OSRD 702. G. B. Kistiakowsky, "The heats of combustion of explosives". (15 July 1942) CONFIDENTIAL.

86. OSRD 5306. G. Stegeman, "Heat of combustion of explosive substances". (4 July 1945) CONFIDENTIAL.

87. G. S. Parks and G. E. Moore, J. Chem. Phys., 7, 1066 (1939). "The heat of combustion of isopropanol".

88. G. S. Parks, T. J. West, B. F. Naylor, P. S. Fujii and L. A. McClaine, J. Am. Chem. Soc., 68, 2524 (1946). "Thermal data on organic compounds. XXIII. Modern combustion data for 14 hydrocarbons and 5 polyhydroxy alcohols."

89. L. Pauling, "The nature of the chemical bond", Cornell University Press, Ithaca, New York (1940) pp. 47-58.

90. Picatinny Arsenal Laboratory Report 134460 (20 February 1951). CONFIDENTIAL.

91. Picatinny Arsenal Tech. Report 1409 (3 April 1944). "Compounds of high nitrogen content in propellant powders". CONFIDENTIAL

92. Picatinny Arsenal Tech. Report 1694 by O. E. Sheffield (26 May 1948) "Long range basic research leading to the development of ideal propellants. Compounds of high nitrogen content propellant powders". CONFIDENTIAL.

93. Picatinny Arsenal Tech. Report 1740 by W. R. Tomlinson (20 June 1949). "Properties of explosives of military interest". CONFIDENTIAL

94. Picatinny Arsenal Tech. Report 1752 by S. Helf (7 Nov. 1949). "Compounds of high nitrogen content in propellant powders". CONF.

95. Picatinny Arsenal Tech. Report 1795 by T. C. Castorina (30 Dec. 1949). "Long range basic research leading to the development of ideal propellants. Explosive plasticizers for nitrocellulose". CONFIDENTIAL

96. Picatinny Arsenal Tech. Report 1841 by S. Helf, I. Minsky and B. D. Guida (1 October 1951). "Long range basic research leading to the development of superior propellants. Compounds of high nitrogen content in propellant compositions". CONFIDENTIAL

97. J. R. Platt, J. Chem. Phys., 15, 419-420 (1947). "Influence of neighbor bonds on additive bond properties in paraffins".

98. T. M. Polonskii, Nauch. Zapiski Khar'kov Poligraf. Inst., 1940 No. 5, 103-6; Khim. Referat. Zhur., 4, No. 4, 26-7 (1941); C.A., 37, 4618 (1943). "The connection between the parachor values and the heats of combustion".

99. A. Pongratz, S. Bohmert-Suss, and K. Scholtis, Ber., 77, 651 (1944); C.A., 40, 6068 (1946). "Thermochemistry of the benzidine rearrangement".

100. E. J. Prosen, W. H. Johnson and F. D. Rossini, J. Research Nat. Bur. Standards, 36, 455-461 (1946); C.A., 40, 5630 (1946). "Heats of combustion and formation at 25° of the alkylbenzenes through $C_{10}H_{14}$, and of the high normal monoalkylbenzenes".

101. E. J. Prosen, F. W. Maron, and F. D. Rossini, J. Research Nat. Bur. Standards, 42, 269 (1949). "Heat of isomerization of the two butadienes".

102. E. J. Prosen and F. D. Rossini, J. Research Nat. Bur. Standards, 34, 59 (1945). "Heats of formation and combustion of 1,3-butadiene and styrene".

103. E. J. Prosen and F. D. Rossini, J. Research Nat. Bur. Standards, 34, 263-269 (1945). "Heats of combustion and formation of the paraffin hydrocarbons at 25°C."

104. N. A. Puschin, Z. physik. Chem., 124, 16 (1926). "The binary system naphthalene-m-dinitrobenzene".

105. M. Rebek, Monatsh., 73, 57-81 (1940); Sitzber. Akad. Wiss. Wien, Math.-naturw. Klasse. Abt. IIb, 149, 1-25 (1940); C.A., 36, 702 (1942). "Distribution of the heats of formation of organic molecules into bond increments. I. Hydrocarbons".

106. M. Rebek, Monatsh., 73, 259-68 (1941); C.A., 36, 5084 (1942). "Distribution of the heats of formation of organic molecules into bond increments. II. Normal chains and isomers".

107. J. W. Richardson and G. S. Parks, J. Am. Chem. Soc., 61, 3543-3546 (1939). "Thermal data on organic compounds. XIX. Modern combustion data for some non-volatile compounds containing carbon, hydrogen, and oxygen".

108. W. H. Rinkenbach, Ind. Eng. Chem., 18, 1195 (1926).

109. W. H. Rinkenbach, Ind. Eng. Chem., 19, 925-? (1927). "Preparation and properties of diethylene glycol dinitrate".

110. W. H. Rinkenbach, J. Am. Chem. Soc., 52, 116 (1930). "The heats of combustion and formation of aromatic nitro compounds".

111. D. E. Roberts and R. S. Jessup, J. Research Nat. Bur. Standards, 40, 281 (1948); C.A., 42, 5327 (1948). "Heat of combustion of phenyl-beta-naphthylamine (N-phenyl-2-naphthylamine)".

112. J. S. Roberts and H. A. Skinner, Trans. Faraday Soc., 45, 339-357 (1949); C.A., 43, 6479 (1949). "Dissociation energies of carbon bonds, and resonance energies in hydrocarbon radicals".

113. F. D. Rossini, Bur. Standards J. Research, 13, 189 (1934). "Heats of combustion and of formation of the normal aliphatic alcohols in the gaseous and liquid states, and the energies of their atomic linkages".

114. F. D. Rossini, Ind. Eng. Chem., 29, 1424-1430 (1937). "Heats of formation of simple organic molecules".

115. F. D. Rossini, K. S. Pitzer, W. J. Taylor, J. P. Ebert, J. E. Kilpatrick, C. W. Beckett, M. G. Williams, and H. G. Werner, "Selected values of properties of hydrocarbons", National Bureau of Standards, U. S. Government Printing Office, Washington, D.C. (1947).

116. W. A. Roth and K. Isecke, Ber., 77B, 537-539 (1944); C.A., 40, 5328 (1946). "The heats of combustion and formation of tetranitromethane".

117. W. A. Roth and Machaleldt, "Dissertation", Braunschweig (19..).

118. W. A. Roth and E. Rist-Schumacher. Z. Elektrochem., 50, 7-9 (1944); C.A., 38, 6183 (1944). "Thermochemistry of the sulfonic acids and acid chlorides".

119. P. P. Rubtsov and L. A. Server'yanov, J. Russ. Phys.-Chem. Soc., 50, 140-144 (1918); C.A., 18, 14?? (1924). "The heats of combustion and of formation of certain explosive nitro compounds from their elements".

120. L. Ruzicka and P. Schlapfer, Helv. Chim. Acta, 16, 162 (1932); C.A., 27, 3919 (1933). "Carbon rings. XXII. Heats of combustion of high-membered cyclic compounds".

121. D. J. Salley and J. B. Gray, J. Am. Chem. Soc., 70, 2650 (1948). "Heats of combustion of some organic nitrogen compounds". See also: J. Am. Chem. Soc., 71, 5925 (1951)

122. Sarrau and Vieille, Compt. rend., 93, 269 (1881). "Heats of formation of explosives; numerical results".

123. E. Schjanberg, Z. physik. Chem., A 172, 197-233 (1935); C.A., 29, 3589 (1935). "The heat of combustion and refraction data for various chlorine-substituted fatty acids and esters. The relation between chemical constitution, heat of combustion, and molecular refraction".

124. A. Schmidt, Z. ges. Schiess-u. Sprengstoffw., 29, 259-266, 296-301 (1934). "Thermochemical tables for explosive chemistry".

125. M. Simonetta, Chimica e Industria (Milan), 29, 37 (1947); C.A., 41, 7165 (1947). The thermal problem in the chain of reactions between ethylene oxide and methanol".

126. H. A. Skinner and H. D. Springall, Nature, 162, 343-344 (1948); C.A., 43, 10 (1949). L. H. Long, Nature, 162, 344-345 (1948); C.A., 43, 10 (1949). "Definitions of bond energy in physical chemistry".

127. M. Souders, C. S. Matthews, and C. O. Hurd, Ind. Eng. Chem., 41, 1048-1055 (1949). "Entropy and heat of formation of hydrocarbon vapors".

128. Solid Propellant Information Agency, SPIA/M3 Propellant Powder Ingredients Manual (1951, unpublished).

128-1. Determined at Naval Powder Factory.
128-2. Determined at Aerojet Engineering Corp.
128-3. Data given by British Advisory Council reports.
128-4. Determined by Picatinny Arsenal.

129. R. Spitzer and H. M. Huffman, J. Am. Chem. Soc., 69, 211 (1947). "Heats of combustion of cyclopentane, cyclohexane, cycloheptane and cyclooctane".

130. British Ministry of Supply Report AC-7048 (July 1944) by H. D. Springall and E. Roberts. "On the calculation of heats of formation, and of the explosive powers of compounds from bond, resonance, and "group" energies". BRITISH SECRET

131. A. Stern and G. Klebs, Ann., 500, 91-108 (1932); C.A., 27, 1346 (1933). "Application of calorimetry to pyrroles and pyrrole dyes. II. Calorimetric determination of simple and multiple-nucleus pyrrole derivatives".

132. A. Stern and G. Klebs, Ann., 504, 287 (1933); C.A., 27, 4796. "Application of calorimetry to pyrroles and pyrrole dyes. III. Calorimetric determination of simple and polynucleated pyrrole derivatives".

133. M. V. Sullivan and H. Hunt. J. Phys. and Colloid Chem., 53, 497 (1949). "Heats of combustion, IV. The heats of combustion of five aromatic amines".

134. S. Sunner, Svensk Kem. Tid., 58, 71-81 (1946); C.A., 40, 3972 (1946). "Determination of combustion heats of organosulfur compounds."

135. V. Swyentoslavskii, Z. physik. Chem., 72, 49-83 (1910); C.A., 4, 2101 (1910). "Thermochemical investigations of organic compounds. III. Nitrogen compounds". Also given by same author in J. Russ. Phys.-Chem. Soc., 41, 387-429 (1909); C.A., 6, 1907 (1911), and J. Russ. Phys.-Chem. Soc., 41, 920-925 (1909); C.A., 5, 1414 (1911).

136. F. Swarts, Rec. trav. chim., 32, 59-89 (1913). "Heat of formation of some organic fluorine compounds".

137. F. Swarts, Rec. trav. chim., 33, 281-98 (1914); Bull. acad. roy. belg., 1914, 18-44; C.A., 9, 445 (1915). "The heat of combustion of some aromatic nitro derivatives".

138. F. Swarts, J. chim. phys., 17, 3-70 (1919). "Thermochemical studies on organic fluorine compounds".

139. W. Swietoslawski and J. Bobinska, Roczniki Chem., 9, 723 (1929); C.A., 24, 1790 (1930). "The heats of combustion of camphor, azobenzene, and hydrazobenzene".

140. J. Taylor and C. R. L. Hall, J. Phys. Coll. Chem., 51, 593 (1947). "Determination of the heat of combustion of nitroglycerin and the thermochemical constants of nitrocellulose".

141. J. Taylor, C. R. L. Hall, and H. Thomas, J. Phys. and Colloid Chem., 51, 580-592 (1947); C.A., 41, 3967 (1947). "The thermochemistry of propellant explosives".

142. A. Tettamanzi and N. Arnaldi, Atti accad. sci. Torino, Classe sci. fis. mat. nat., 77, 278-281 (1942); Chem. Zentr., 1943, I, 1848-1849; C. A., 38, 3841 (1944). "Preparation of hexanitrosorbitol and it explosive properties".

143. K. Tomioka and Takahashi, Rep. Res. Dep. Nav. Expl. 1934, p. 122. Tables An. In. de Constantes (1931-1934) 1st Part, Vol. XI, p. 12-51. (As cited by Burlot, Ref. 27).

144. P. E. Verkade and J. Coops, Rec. trav. chim., 46, 903-917 (1927); C.A., 22, 571 (1928). "Calorimetric researches XIV. Heats of combustion of successive members of homologous series: the normal primary aliphatic alcohols".

145. P. E. Verkade and J. Coops, Jr., Proc. Acad. Sci. Amsterdam, 36, 76-87 (1933); C.A., 27, 3134 (1933). "Alternations in the properties of monoalkylmalonic acids. Halkin's views concerning the alternation phenomena".

146. P. E. Verkade, J. Coops, and H. Hartman, Rec. trav. chim., 45, 585-606 (1926); C.A., 21, 1216 (1927). "Calorimetric researches. XIII. Heats of combustion of successive terms of homologous series".

147. P. E. Verkade and H. Hartman, Rec. trav. chim., 52, 945-68 (1933); C.A., 28, 30 (1934). "Calorimetric investigations. XXI. Heats of combustion of methyl-, ethyl- and phenyl-substituted succinic acids and of their anhydrides ... (a) experimental data".

148. P. E. Verkade, H. Hartman, and J. Coops, Rec. trav. chim., 45, 373-393 (1926); C.A., 20, 2937 (1926). "Calorimetric researches. X. Heats of combustion of successive terms of homologous series: dicarboxylic acids of the oxalic acid series".

149. G. Waddington, J. W. Knowlton, D. W. Scott, G. D. Oliver, S. S. Todd, W. N. Hubbard, J. C. Smith and H. H. Huffman, J. Am. Chem. Soc., 71, 797 (1949). "Thermodynamic properties of thiophene".

150. A. D. Walsh, Trans. Faraday Soc., 43, 60-77 (1947); C.A., 41, 4978 (1947). "Remarks on the strengths of bonds".

151. G. W. Wheland, "The theory of resonance", John Wiley and Sons, New York (1944) pp. 52-87.

152. H. Wieland, K. Heymann, T. Tsatsas, D. Juchum, G. Varvoglis, G. Labriola, O. Dobbelstein, and H. S. Boyd-Barrett, Ann., 514, 145-181 (1934); C.A., 29, 1800 (1935). "Occurrence of free radicals in chemical reactions. VIII"

153. J. B. Willis, Trans. Faraday Soc., 43, 97-102 (1947); C.A., 41, 5008 (1947). "Heats of combustion of some organic bases and their salts. The resonance energy of acridine and phenazine".

154. P. H. Wise, K. T. Serijan, and I. A. Goodman, Technical Note 2081 for National Advisory Committee for Aeronautics (Copied for OCO 12 September, 1950). "Correlation of physical properties with molecular structure for dicyclic hydrocarbons. I. 2-n-Alkylbiphenyls, 1,1-diphenylalkane, α,ω-diphenylalkane, 1,1-dicyclohexylalkane, and α,ω-dicyclohexylalkane series". Also appears as: K. T. Serijan and P. H. Wise, J. Am. Chem. Soc., 73, 4766-4769 (1951). "Dicyclic hydrocarbons. III. Diphenyl- and dicyclohexylalkanes through C_{18}".

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1. Glossary of Terms and Symbols

A functional group is any substituent for a hydrogen of a normal paraffin.

A monofunctional compound is one containing a single functional group.

A polyfunctional compound contains more than one functional group which may be alike or different.

A homofunctional compound contains only one functional type and may be either mono or polyfunctional.

A heterofunctional compound contains more than one functional type and is necessarily polyfunctional.

Molar oxygen balance is equal to the atoms of external oxygen required to complete the combustion of a compound to carbon dioxide, water, and nitrogen (and to hydrohalide and sulfur dioxide when X and S are present).

Q_C = heat of combustion (H_2O liquid), heat evolved; H_C of Part II (Ref. 70); $-\Delta H$ of Lewis and Randall.

superscript p = constant pressure as in Q_C^p

superscript v = constant volume as in Q_C^v

x = oxygen balance on a molar basis

x' = x divided by number of homofunctional groups

$y = Q_C^p$

y' = (Q_C^p - 5.7) divided by number of homofunctional groups

a = intercept of a homologous series; the value of y when x = 0. For paraffins the intercept is 5.7.

b = slope of a homologous series, or $\frac{y'_2 - y'_1}{x'_2 - x'_1}$. For normal paraffins (liq) the slope is 52.08.

a' = (a - 5.7) for liquid and solid state, (a - 5.5) for gas state; the value of y' when x' = 0.

b' = (52.08 - b) for liquid and solid states, (52.48 - b) for gas state.

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J. Heat of Combustion Data

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Heat of Combustion Data (cont'd)

TABLE 61

NORMAL PARAFFINS (liquid)

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	G_c°, KCAL/MOLE OBSERVED	G_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_3H_8	Propane	44.09	10	-362.9	525.6	526.5			115-1
	C_4H_{10}	n-Butane	58.12	13	-357.9	682.8	682.7			115-1
	C_5H_{12}	n-Pentane	72.15	16	-354.8	838.8	839.0			115-1
	C_6H_{14}	n-Hexane	86.17	19	-352.8	995.0	995.2			115-1
	C_7H_{16}	n-Heptane	100.20	22	-351.3	1151.3	1151.4			115-1
	C_8H_{18}	n-Octane	114.22	25	-350.2	1307.5	1307.7			115-1
	C_9H_{20}	n-Nonane	128.25	28	-349.3	1463.8	1463.9			115-1
	$C_{10}H_{22}$	n-Decane	142.28	31	-348.6	1620.1	1620.1			115-1
	$C_{11}H_{24}$	n-Undecane	156.30	34	-348.0	1776.3	1776.4			115-1
	$C_{12}H_{26}$	n-Dodecane	170.33	37	-347.6	1932.6	1932.6			115-1
	$C_{13}H_{28}$	n-Tridecane	184.35	40	-347.2	2088.9	2088.9			115-1
	$C_{14}H_{30}$	n-Tetradecane	198.38	43	-346.8	2245.1	2245.3			115-1
	$C_{15}H_{32}$	n-Pentadecane	212.41	46	-346.5	2401.4	2401.4			115-1
	$C_{16}H_{34}$	n-Hexadecane	226.43	49	-346.2	2557.6	2557.6			115-1
	$C_{17}H_{36}$	n-Heptadecane	240.46	52	-346.0	2713.9	2713.8			115-1
	$C_{18}H_{38}$	n-Octadecane	254.48	55	-345.8	2870.2	2870.1			115-1
	$C_{19}H_{40}$	n-Nonadecane	268.51	58	-345.6	3026.4	3026.3			115-1
	$C_{20}H_{42}$	n-Eicosane	282.54	61	-345.4	3182.7	3182.6			115-1
		$y = 5.67 + 52.08x$						$\Sigma x = 6[illegible].0$ $\Sigma y = 33,361.2$ $\Sigma xy = 1,412,[illegible]38.00$ $\Sigma x^2 = 27,0[illegible].00$ $n = 18$		
	CH_4	Methane	16.04	4	-399.0	-	214.0			115-1
	C_2H_6	Ethane	30.07	7	-372.5	-	370.2			115-1

TABLE 62

NORMAL PARAFFINS (gas)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	G_c°, KCAL/MOLE OBSERVED	G_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_2H_6	Ethane	30.07	7	-372.5	372.82	372.[illegible]			115-1
	C_3H_8	Propane	44.09	10	-362.9	530.61	530.[illegible]			115-1
	C_4H_{10}	n-Butane	58.12	13	-357.9	687.98	687.7			115-1
	C_5H_{12}	n-Pentane	72.15	16	-354.8	845.16	845.2			115-1
	C_6H_{14}	n-Hexane	86.17	19	-352.8	1002.57	1002.6			115-1
	C_7H_{16}	n-Heptane	100.20	22	-351.3	1160.01	1160.1			115-1
	C_8H_{18}	n-Octane	114.22	25	-350.2	1317.45	1317.5			115-1
	C_9H_{20}	n-Nonane	128.25	28	-349.3	1474.90	1474.9			115-1
	$C_{10}H_{22}$	n-Decane	142.28	31	-348.6	1632.34	1632.4			115-1
	$C_{11}H_{24}$	n-Undecane	156.30	34	-348.0	1789.78	1789.8			115-1
	$C_{12}H_{26}$	n-Dodecane	170.33	37	-347.6	1947.23	1947.3			115-1
	$C_{13}H_{28}$	n-Tridecane	184.35	40	-347.2	2104.67	2104.7			115-1
	$C_{14}H_{30}$	n-Tetradecane	198.38	43	-346.8	2262.11	2262.1			115-1
	$C_{15}H_{32}$	n-Pentadecane	212.41	46	-346.5	2419.55	2419.6			115-1
	$C_{16}H_{34}$	n-Hexadecane	226.43	49	-346.2	2577.00	2577.0			115-1
	$C_{17}H_{36}$	n-Heptadecane	240.46	52	-346.0	2734.44	2734.5			115-1
	$C_{18}H_{38}$	n-Octadecane	254.48	55	-345.8	2891.88	2891.9			115-1
	$C_{19}H_{40}$	n-Nonadecane	268.51	58	-345.6	3049.33	3049.3			115-1
	$C_{20}H_{42}$	n-Eicosane	282.54	61	-345.4	3206.77	3206.8			115-1
		$y = 5.50 + 52.48x$						$\Sigma x = 646.0$ $\Sigma y = 34,006.6$ $\Sigma xy = 1,425,435.43$ $\Sigma x^2 = 27,07[illegible].0$ $n = 19$		
	CH_4	Methane	16.04	4		212.80	215.4			115-1

TABLE 63

NORMAL PARAFFINS—HEAT OF VAPORIZATION AT 25°C

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_v^p, OBSERVED[a] KCAL/MOLE	Q_v^p, OBSERVED[a] CAL/GRAM	Y'	X'	REF.
	C_3H_8	n-Propane	44.09			3.8	86.7			115-1
	C_4H_{10}	n-Butane	58.12			5.1	88.4			115-1
	C_5H_{12}	n-Pentane	72.15			6.4	88.1			115-1
	C_6H_{14}	n-Hexane	86.17			7.6	87.7			115-1
	C_7H_{16}	n-Heptane	100.20			8.7	87.2			115-1
	C_8H_{18}	n-Octane	114.22			9.9	86.8			115-1
	C_9H_{20}	n-Nonane	128.25			11.1	86.5			115-1
	$C_{10}H_{22}$	n-Decane	142.28			12.3	86.[illegible]			115-1
	$C_{11}H_{24}$	n-Undecane	156.30			13.5	86.[illegible]			115-1
	$C_{12}H_{26}$	n-Dodecane	170.33			14.6	85.9			115-1
	$C_{13}H_{28}$	n-Tridecane	184.35			15.8	85.9			115-1
	$C_{14}H_{30}$	n-Tetradecane	198.38			17.0	85.7			115-1
	$C_{15}H_{32}$	n-Pentadecane	212.41			18.2	85.6			115-1
	$C_{16}H_{34}$	n-Hexadecane	226.43			19.4	85.5			115-1
	$C_{17}H_{36}$	n-Heptadecane	240.46			20.5	85.4			115-1
	$C_{18}H_{38}$	n-Octadecane	254.49			21.7	85.3			115-1
	$C_{19}H_{40}$	n-Nonadecane	268.51			22.9	85.3			115-1
	$C_{20}H_{42}$	n-Eicosane	282.54			24.1	85.3			115-1
						AVERAGE	86.3			
	C_2H_6	Ethane	30.07			2.6	(Calc.)			115-1
	CH_4	Methane	16.04			1.4	(Calc.)			115-1

a) Q_c^p (g) - Q_c^p (l)

These values were subtracted from Q_c^p (gas) to give Q_c^p (liq) for cycloparaffins, olefins and acetylenes where necessary to obtain data given in Tables 67, 68, 71, 73, and 75.

TABLE 64

BRANCHED PARAFFINS (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_4H_{10}	2-Methylpropane	58.12	13	-357.9	681.6	680.2	679.9	13	115-2
	C_5H_{12}	2-Methylbutane	72.15	16	-354.8	837.3	836.7	831.6	16	115-2
		2,2-Dimethylpropane	•	•	•	835.2	•	829.5	16	115-2
	C_6H_{14}	2-Methylpentane	86.17	19	-352.8	993.7		988.0	19	115-2
	•	3-Methylpentane	•	•	•	994.3	•	988.6	19	115-2
	•	2,3-Dimethylbutane	•	•	•	993.1	•	987.4	19	115-2
	•	2,2-Dimethylbutane	•	•	•	991.5	•	985.8	19	115-2
	C_7H_{16}	2-Methylhexane	100.20	22	-351.3	1150.0	1149.7	1144.3	22	115-2
	•	3-Methylhexane	•	•	•	1150.6	•	1144.9	22	115-2
	•	3-Ethylpentane	•	•	•	1151.1	•	1145.4	22	115-2
	•	2,3-Dimethylpentane	•	•	•	1149.1	•	1143.4	22	115-2
	•	2,4-Dimethylpentane	•	•	•	1148.7	•	1143.0	22	115-2
	•	2,2-Dimethylpentane	•	•	•	1147.9	•	1142.2	22	115-2
	•	3,3-Dimethylpentane	•	•	•	1148.8	•	1143.1	22	115-2
	•	2,2,3-Trimethylbutane	•	•	•	1148.3	•	1142.6	22	115-2
	C_8H_{18}	2-Methylheptane	114.22	25	-350.2	1306.3	1306.2	1300.6	25	115-2
	•	3-Methylheptane	•	•	•	1306.9	•	1301.2	25	115-2
	•	4-Methylheptane	•	•	•	1307.1	•	1301.4	25	115-2
	•	3-Ethylhexane	•	•	•	1307.4	•	1301.7	25	115-2
	•	2,3-Dimethylhexane	•	•	•	1306.9	•	1301.2	25	115-2
	•	2,4-Dimethylhexane	•	•	•	1305.8	•	1300.1	25	115-2
	•	2,5-Dimethylhexane	•	•	•	1305.0	•	1299.3	25	115-2
	•	3,4-Dimethylhexane	•	•	•	1307.0	•	1301.3	25	115-2
	•	2-Methyl-3-ethylpentane	•	•	•	1307.6	•	1301.9	25	115-2
	•	2,3,4-Trimethylpentane	•	•	•	1306.3	•	1300.6	25	115-2
	•	2,2-Dimethylhexane	•	•	•	1304.6	•	1298.9	25	115-2
	•	3,3-Dimethylhexane	•	•	•	1305.7	•	1300.0	25	115-2
	•	3-Methyl-3-ethylpentane	•	•	•	1306.8	•	1301.1	25	115-2

$y' = -3.74 + 52.17x'$

$\Sigma x' = 622.0$
$\Sigma y' = 32,345.0$
$\Sigma x'y' = 734,418.0$
$\Sigma x'^2 = 14,122.0$
$n = 28$

TABLE 65

CYCLOPROPANES (liquid and solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	C_3H_6	Cyclopropane	42.08	9	-342.2	[illegible]	[illegible]	[illegible]	9	60
	$C_5H_6O_4$	1,1-Cyclopropanedicarboxylic acid (s)	130.10	"	-110.7	482.9	481.8	484.9	"	55-187
	"	cis-1,2- " (s)	"	"	"	483.9	"	485.9	9	55-187
	$C_7H_6O_8$	1,1,2,2-Cyclopropanetetracarboxylic acid (s)	218.12	"	-66.0	482.7	476.3	482.2	9	55-187
	$C_4H_6O_2$	Cyclopropanecarboxylic acid	86.09	"	-167.3	477.3	485.4	477.7	9	55-175
		"	"	"	"	481.7	"	482.1	9	55-215
	C_5H_8O	Cyclopropyl methyl ketone	84.11	13	-247.3	691.4	700.3	6[illegible].7	13	55-215
	$C_5H_{10}O_2$	Cyclopropanedimethanol	104.13	"	-203.7	707.6	714.9	684.3	13	55-215
	$C_{11}H_{14}O_8$	Tetramethyl 1,1,2,2-cyclopropanetetracarboxylate (s)	274.22	21	-122.5	1169.7	1164.4	1112.5	21	55-187

$y' = 16.22 + 51.95x'$

$\Sigma x' = 101.0$
$\Sigma y' = 5,392.[illegible]$
$\Sigma x'y' = 67,354.1$
$\Sigma x'^2 = 1265.0$
$n = 9$

TABLE 66

CYCLOBUTANES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	$C_5H_8O_2$	Cyclobutanecarboxylic acid	100.11	12	-191.8	641.0	638.4	637.2	12	55-175
		"	"	"	"	639.2	"	637.4	12	55-213
	$C_5H_{10}O$	Cyclobutanemethanol	86.13	14	-260.1	747.8	755.2	731.6	14	55-215
	$C_6H_{10}O_2$	Methyl cyclobutanecarboxylate	114.14	15	-210.3	809.1	808.7	793.6	15	55-215
	$C_6H_{10}O$	Cyclobutyl methyl ketone	98.14	16	-260.9	856.8	851.5	848.6	16	55-215
		$y' = 10.26 + 52.15x'$								
	$C_6H_8O_4$	1,1-Cyclobutanedicarboxylic acid (s)	144.12	12	-133.2	642.0	634.0			55-187
	"	cis-1,2- " (s)	"	"	"	642.1	-			55-187
	"	1,3- " (s)	"	"	"	639.4	"			55-243
	C_5H_{10}	Methylcyclobutane	70.13	15	-342.2	7[illegible]2	759.9			55-215

$\Sigma x' = 69.0$
$\Sigma y' = 3652.4$
$\Sigma x'y' = 51,071.2$
$\Sigma x'^2 = 965.0$
$n = 5$

TABLE 67

NORMAL ALKYL CYCLOPENTANES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	C_5H_{10}	Cyclopentane	70.13	15	-342.2	785.5	785.1	780.8	15	115-3
	C_6H_{12}	Methylcyclopentane	84.16	18	"	941.1	941.5	935.4	18	115-3
	C_7H_{14}	Ethylcyclopentane	98.18	21	"	1097.5	1097.7	1091.8	21	115-3
	C_8H_{16}	n-Propylcyclopentane	112.21	24	"	1253.7	1254.0	1248.0	24	115-3
	C_9H_{18}	n-Butylcyclopentane	126.23	27	"	1410.1	1410.2	1404.4	27	115-3
	$C_{10}H_{20}$	n-Pentylcyclopentane	140.26	30	"	1566.4*	1566.4	1560.7	30	115-3
	$C_{11}H_{22}$	n-Hexylcyclopentane	154.29	33	"	1722.7*	1722.7	1717.[illegible]	33	115-3
	$C_{12}H_{24}$	n-Heptylcyclopentane	168.31	36	"	1878.9*	1878.9	1873.2	36	115-3
	$C_{13}H_{26}$	n-Octylcyclopentane	182.34	39	"	2035.2*	2035.2	2029.5	39	115-3
	$C_{14}H_{28}$	n-Nonylcyclopentane	196.36	42	"	2191.4*	2191.4	2185.7	42	115-3
	$C_{15}H_{30}$	n-Decylcyclopentane	210.39	45	"	2347.6*	2347.6	2341.9	45	115-3
	$C_{16}H_{32}$	n-Undecylcyclopentane	224.42	48	"	2503.8*	2503.9	2498.1	48	115-3
	$C_{17}H_{34}$	n-Dodecylcyclopentane	238.[illegible]	51	"	2660.[illegible]*	2660.1	2654.5	51	115-3
	$C_{18}H_{36}$	n-Tridecylcyclopentane	252.47	54	"	2816.3*	2816.4	2810.6	54	115-3
	$C_{19}H_{38}$	n-Tetradecylcyclopentane	266.[illegible]	57	"	2972.5*	2972.6	2966.8	57	115-3
	$C_{20}H_{40}$	n-Pentadecylcyclopentane	280.52	60	"	3128.6*	3128.[illegible]	3123.1	60	115-3

$y' = -1.67 + 52.08x'$

*Corrected to liquid from gas values given in Reference 115 using heat of vaporization = 86.3 cal/g as in Table 53.

$\Sigma x' = 600.0$
$\Sigma y' = 31,221.5$
$\Sigma x'y' = 1,330,154.7$
$\Sigma x'^2 = 2[illegible],560.0$
$n = 16$

TABLE 68

NORMAL ALKYL CYCLOHEXANES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_6H_{12}	Cyclohexane	84.16	18	-342.2	936.9	935.7	931.2	18	115-4
	C_7H_{14}	Methylcyclohexane	98.18	21	"	1091.1	1091.9	1086.4	21	115-4
	C_8H_{16}	Ethylcyclohexane	112.21	24	"	1248.[illegible]	[illegible]	1241.5	24	115-4
	C_9H_{18}	n-Propylcyclohexane	126.23	27	"	1404.3	1404.4	1398.6	27	115-4
	$C_{10}H_{20}$	n-Butylcyclohexane	140.26	30	"	1560.6	1560.6	1555.1	30	115-4
	$C_{11}H_{22}$	n-Pentylcyclohexane	154.29	33	"	1716.9*	1716.9	1711.2	33	115-4
	$C_{12}H_{24}$	n-Hexylcyclohexane	168.31	36	"	1873.1*	1873.1	1867.4	36	115-4
	$C_{13}H_{26}$	n-Heptylcyclohexane	182.34	39	"	2029.4*	2029.4	2023.7	39	115-4
	$C_{14}H_{28}$	n-Octylcyclohexane	196.36	42	"	2185.6*	2185.6	2179.9	42	115-4
	$C_{15}H_{30}$	n-Nonylcyclohexane	210.39	45	"	2341.8*	2341.8	2336.1	45	115-4
	$C_{16}H_{32}$	n-Decylcyclohexane	224.42	48	"	2498.0*	2498.1	2492.3	48	115-4
	$C_{17}H_{34}$	n-Undecylcyclohexane	238.44	51	"	2654.2*	2654.3	2648.5	51	115-4
	$C_{18}H_{36}$	n-Dodecylcyclohexane	252.47	54	"	2810.5*	2810.5	2804.8	54	115-4
	$C_{19}H_{38}$	n-Tridecylcyclohexane	266.49	57	"	2966.7*	2966.8	2961.0	57	115-4
	$C_{20}H_{40}$	n-Tetradecylcyclohexane	280.52	60	"	3123.0*	3123.0	3117.3	60	115-4

$y' = -7.43 + 52.08x'$

$\Sigma x' = 585.0$
$\Sigma y' = 30,355.0$
$\Sigma x'y' = 1,315,068.90$
$\Sigma x'^2 = 25,335.0$
$n = 15$

*Corrected to liquid from gas values given in Reference 115 by subtracting 66.3 cal/g. as [illegible]

TABLE 69

CYCLOHEPTANES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_7H_{12}O$	Cycloheptanone	112.17	19	-271.0	936.7	935.4	932.1	19	55-215
	C_7H_{12}	Cycloheptene	96.17	20	-332.7	1049.9	1050.6	1030.2	20	55-215
	$C_7H_{14}O$	Cycloheptanol	114.18	"	-280.3	1050.2	1060.3	1048.8	20	55-215
	C_7H_{14}	Cycloheptane	98.11	21	-342.5	1099.1	1095.7	1093.4	21	129
	$C_8H_{14}O_2$	Cycloheptanecarboxylic acid (s)	142.19	"	-236.3	1087.9	1091.7	1086.2	21	55-215
	C_8H_{16}	Methylcycloheptane	112.21	24	-342.2	1244.5	1249.0	1238.8	24	55-215
	$C_9H_{18}O$	Cycloheptyl methyl carbinol	142.32	26½	-292.3	1342.2	1344.2	1343.4	26	55-215
	C_9H_{18}	Ethylcycloheptane	126.23	27	-342.2	1406.8	1402.2	1401.1	27	55-215
		$y' = 17.12 + 51.06x'$								
	$C_9H_{16}O$	Cycloheptyl methyl ketone	140.22	25	-285.3	1278.3	1280.8	-	-	55-215

$\Sigma x' = 178.0$
$\Sigma y' = 9231.0$
$\Sigma x'y' = 208,633.[illegible]$
$\Sigma x'^2 = 4026.0$
$n = 8$

TABLE 70

OTHER SATURATED ALICYCLIC HYDROCARBONS

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_9H_{16}O_2$	Cyclooctanecarboxylic acid (1)	152.23	21	-235.3	1089.2 (?)				55-215
	C_8H_{16}	Cyclooctane (1)	112.21	24	-342.2	1258.4				129
	$C_{10}H_{20}$	Cyclodecane (1)	140.26	30	"	1570.8				46
	$C_{15}H_{30}$	Cyclopentadecane (s)	210.[illegible]	45	"	2360				120
	$C_{17}H_{34}$	Cycloheptadecane (s)	238.44	51	"	2678				120
	$C_{30}H_{60}$	Cyclotriacontane (s)	420.78	90	"	4674				120

TABLE 71

NORMAL OLEFINS (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED*	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_3H_6	Propene	42.08	9	-342.2	[illegible]	[illegible]	487.7	9	115-9
	C_4H_8	1-Butene	56.10	12	"	644.9	644.7	639.7	12	115-9
	C_5H_{10}	1-Pentene	70.13	15	"	801.8	800.9	795.1	15	115-9
	C_6H_{12}	1-Hexene	84.16	18	"	957.0	957.1	951.3	18	115-9
	C_7H_{14}	1-Heptene	98.18	21	"	1113.2	[illegible]	1107.5	21	115-9
	C_8H_{16}	1-Octene	112.21	24	"	1269.4	1267.6	1263.1	24	115-9
	C_9H_{18}	1-Nonene	126.23	27	"	1425.7	1425.8	1420.0	27	115-9
	$C_{10}H_{20}$	1-Decene	140.26	30	"	1581.9	1582.0	1576.2	30	115-9
	$C_{11}H_{22}$	1-Undecene	154.29	33	"	1738.1	1738.2	1732.4	33	115-9
	$C_{12}H_{24}$	1-Dodecene	168.31	36	"	1894.4	1894.4	[illegible]	36	115-9
	$C_{13}H_{26}$	1-Tridecene	182.34	39	"	2050.6	2050.6	2044.9	39	115-9
	$C_{14}H_{28}$	1-Tetradecene	196.36	42	"	2206.8	2206.8	2201.1	42	115-9
	$C_{15}H_{30}$	1-Pentadecene	210.39	45	"	2363.1	2363.0	2357.4	45	115-9
	$C_{16}H_{32}$	1-Hexadecene	224.42	48	"	2519.3	2519.2	2513.6	48	115-9
	$C_{17}H_{34}$	1-Heptadecene	238.44	51	"	2675.6	2675.4	2669.9	51	115-9
	$C_{18}H_{36}$	1-Octadecene	252.47	54	"	2831.8	2831.7	[illegible]	54	115-9
	$C_{19}H_{38}$	1-Nonadecene	266.49	57	"	2988.0	2987.8	2982.3	57	115-9
	$C_{20}H_{40}$	1-Eicosene	280.52	60	"	3144.2	3144.1	3138.5	60	115-9
		y' = 14.20 + 5[illegible].07x'						Σx' = [illegible] Σy' = 37,550.6 Σx'y' = 1,351,447.80 Σx'² = 25,785.0 n = 18		
	C_2H_4	Ethylene	28.05	6	-342.2	-	332.3	-	-	115-9
		*Corrected to liquid state from gas values given in Reference 115 by subtracting 86.3 cal/g as in Table 6[illegible].								

TABLE 72

NORMAL OLEFINS (gas)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_3H_6	Propene	42.08	9	-342.2	[illegible]	491.97	486.49		115-9
	C_4H_8	1-Butene	56.10	12	"	649.76	649.75	644.26		115-9
	C_5H_{10}	1-Pentene	70.13	15	"	806.85	806.85	801.35		115-9
	C_6H_{12}	1-Hexene	84.16	18	"	964.76	964.79	[illegible]		115-9
	C_7H_{14}	1-Heptene	98.18	21	"	1121.69	1121.73	1116.19		115-9
	C_8H_{16}	1-Octene	112.21	24	"	1279.13	1279.17	1273.63		115-9
	C_9H_{18}	1-Nonene	126.23	27	"	1436.58	1436.61	1431.08		115-9
	$C_{10}H_{20}$	1-Decene	140.26	30	"	1594.02	1594.05	1588.52		115-9
	$C_{11}H_{22}$	1-Undecene	154.29	33	"	1751.46	1751.49	1745.96		115-9
	$C_{12}H_{24}$	1-Dodecene	168.31	36	"	1908.91	1908.93	1903.41		115-9
	$C_{13}H_{26}$	1-Tridecene	182.34	39	"	2066.35	2066.37	2060.85		115-9
	$C_{14}H_{28}$	1-Tetradecene	196.36	42	"	2223.79	2223.81	2218.29		115-9
	$C_{15}H_{30}$	1-Pentadecene	210.39	45	"	2381.23	2381.25	2375.73		115-9
	$C_{16}H_{32}$	1-Hexadecene	224.42	48	"	2538.68	2538.69	2533.18		115-9
	$C_{17}H_{34}$	1-Heptadecene	238.44	51	"	2696.13	2696.13	2690.63		115-9
	$C_{18}H_{36}$	1-Octadecene	252.47	54	"	2853.57	2853.57	2848.07		115-9
	$C_{19}H_{38}$	1-Nonadecene	266.49	57	"	3011.01	3011.01	3005.51		115-9
	$C_{20}H_{40}$	1-Eicosene	280.52	60	"	3168.45	3168.45	3162.95		115-9
		y' = 14.15 + 52.40x'						Σx' = 621.0 Σy' = 37,441.06 Σx'y' = 1,341,977.57 Σx'² = 25,785.0 n = 18		
	C_2H_4	Ethene	28.05	6	-342.2	337.2	334.5	-		115-9

TABLE 73

BRANCHED OLEFINS (liquid)

ALT NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^v, KCAL/MOLE OBSERVED*	Q_c^v, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_4H_8	cis-2-Butene	56.10	12	-342.2	643.2	642.1			115-5
	"	trans-2-Butene	"	"	"	642.2	"			115-5
	"	2-Methylpropene	"	"	"	641.2	"			115-5
	C_5H_{10}	cis-2-Pentene	70.13	15	"	799.4	798.6			115-5
	"	trans-2-Pentene	"	"	"	798.4	"			115-5
	"	2-Methyl-1-butene	"	"	"	792.2	"			115-5
	"	3-Methyl-1-butene	"	"	"	799.0	"			115-5
	"	2-Methyl-2-butene	"	"	"	795.8	"			115-5
	C_6H_{12}	cis-2-Hexene	84.16	18	"	955.6	955.0			115-5
	"	trans-2-Hexene	"	"	"	954.6	"			115-5
	"	cis-3-Hexene	"	"	"	955.6	"			115-5
	"	trans-3-Hexene	"	"	"	954.6	"			115-5
	"	2-Methyl-1-pentene	"	"	"	953.6	"			115-5
	"	3-Methyl-1-pentene	"	"	"	956.1	"			115-5
	"	4-Methyl-1-pentene	"	"	"	955.5	"			115-5
	"	2-Methyl-2-pentene	"	"	"	952.2	"			115-5
	"	cis-3-Methyl-2-pentene	"	"	"	952.8	"			115-5
	"	trans-3-Methyl-2-pentene	"	"	"	952.6	"			115-5
	"	cis-4-Methyl-2-pentene	"	"	"	953.9	"			115-5
	"	trans-4-Methyl-2-pentene	"	"	"	952.9	"			115-5
	"	2-Ethyl-1-butene	"	"	"	954.2	"			115-5
	"	2,3-Dimethyl-1-butene	"	"	"	952.3	"			115-5
	"	3,3-Dimethyl-1-butene	"	"	"	952.9	"			115-5
	"	2,3-Dimethyl-2-butene	"	"	"	951.2	"			115-5
	C_7H_{14}	cis-2-Heptene	98.18	21	"	1112.0	1111.6			115-5
	"	trans-2-Heptene	"	"	"	1111.0	"			115-5
	"	cis-3-Heptene	"	"	"	1112.0	"			115-5
	"	trans-3-Heptene	"	"	"	1111.0	"			115-5
	"	2-Methyl-1-hexene	"	"	"	1110.0	"			115-5
	"	3-Methyl-1-hexene	"	"	"	1112.5	"			115-5
	"	4-Methyl-1-hexene	"	"	"	1112.5	"			115-5
	"	5-Methyl-1-hexene	"	"	"	1112.9	"			115-5
	"	2-Methyl-2-hexene	"	"	"	1108.6	"			115-5
	"	cis-3-Methyl-2-hexene	"	"	"	1109.7	"			115-5
	"	trans-3-Methyl-2-hexene	"	"	"	1109.2	"			115-5
	"	cis-4-Methyl-2-hexene	"	"	"	1110.9	"			115-5
	"	trans-4-Methyl-2-hexene	"	"	"	1109.9	"			115-5
	"	cis-5-Methyl-2-hexene	"	"	"	1110.3	"			115-5
	"	trans-5-Methyl-2-hexene	"	"	"	1109.3	"			115-5
	"	cis-2-Methyl-3-hexene	"	"	"	1110.3	"			115-5
	"	trans-2-Methyl-3-hexene	"	"	"	1109.2	"			115-5
	"	cis-3-Methyl-3-hexene	"	"	"	1109.7	"			115-5
	"	trans-3-Methyl-3-hexene	"	"	"	1109.3	"			115-5
	"	2-Ethyl-1-pentene	"	"	"	1110.6	"			115-5
	"	3-Ethyl-1-pentene	"	"	"	1113.1	"			115-5
	"	2,3-Dimethyl-1-pentene	"	"	"	1109.0	"			115-5
	"	2,4-Dimethyl-1-pentene	"	"	"	[illegible]	"			115-5
	"	3,3-Dimethyl-1-pentene	"	"	"	1110.3	"			115-5
	"	3,4-Dimethyl-1-pentene	"	"	"	1110.8	"			115-5
	"	4,4-Dimethyl-1-pentene	"	"	"	1109.2	"			115-5
	"	3-Ethyl-2-pentene	"	"	"	1109.6	"			115-5
	"	2,3-Dimethyl-2-pentene	"	"	"	1107.4	"			115-5
	"	2,4-Dimethyl-2-pentene	"	"	"	1106.9	"			115-5
	"	cis-3,4-Dimethyl-2-pentene	"	"	"	1107.6	"			115-5
	"	trans-3,4-Dimethyl-2-pentene	"	"	"	[illegible]	"			115-5
	"	cis-4,4-Dimethyl-2-pentene	"	"	"	1107.6	"			115-5
	"	trans-4,4-Dimethyl-2-pentene	"	"	"	1106.6	"			115-5
	"	3-Methyl-2-ethyl-1-butene	"	"	"	1109.0	"			115-5
	"	2,3,3-Trimethyl-1-butene	"	"	"	1107.6	"			115-5
	C_8H_{16}	Di-i-butylene	112.21	24	"	1266.4	1268.0			11
	$C_{10}H_{20}$	Diamylene	140.26	30	"	1582.2	1581.0			55-65

For branched olefins: $y = 16.2 + 52.16x$

*Corrected to liquid state from gas values given in Reference 115 by subtracting 86.3 cal/g as in Table 63.

TABLE 74

DIOLEFINS (liquid)

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c° KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	C_4H_6	1,2-Butadiene	54.09	11	-325.4	619.6	606.9			101
	"	1,3-Butadiene	"	"	"	602.0	"			104
	C_5H_8	Isoprene	68.11	14	-328.9	755.3	759.9			53
	C_6H_{10}	1,5-Hexadiene	82.14	17	-331.1	918.4	919.3			27
	"	"	"	"	"	936.0	"			61
	"	2,3-Dimethyl-1,3-butadiene	"	"	"	911.7	912.4			61

For n-diolefins: $y = 34.1 + 52.07x$
For branched diolefins: $y = 15.7 + 52.16x$

TABLE 75

ACETYLENES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c° KCAL/MOLE OBSERVED*	CALCULATED	Y'	X'	REF.
	C_3H_4	Propyne	40.06	8	-319.5	469.7	469.6	462.0	8	115-6
	C_4H_6	1-Butyne	54.09	11	-325.4	616.2	615.9	610.5	11	115-6
	C_5H_8	1-Pentyne	68.11	14	-328.9	772.2	772.1	766.5	14	115-6
	C_6H_{10}	1-Hexyne	82.14	17	-331.1	926.4	928.4	922.7	17	115-6
	C_7H_{12}	1-Heptyne	96.17	20	-332.7	1084.6	1084.6	1078.9	20	115-6
	C_8H_{14}	1-Octyne	110.19	23	-334.0	1240.4	1240.8	1235.1	23	115-6
	C_9H_{16}	1-Nonyne	124.22	26	-334.9	1397.0	1397.1	1391.3	26	115-6
	$C_{10}H_{18}$	1-Decyne	138.24	29	-335.6	1553.3	1553.3	1547.6	29	115-6
	$C_{11}H_{20}$	1-Undecyne	152.27	32	-336.2	1709.5	1709.5	1703.9	32	115-6
	$C_{12}H_{22}$	1-Dodecyne	166.30	35	-336.7	1865.4	1865.8	1860.2	35	115-6
	$C_{13}H_{24}$	1-Tridecyne	180.32	38	-337.2	2022.0	2022.0	2016.3	38	115-6
	$C_{14}H_{26}$	1-Tetradecyne	194.35	41	-337.5	2178.2	2178.3	2172.5	41	115-6
	$C_{15}H_{28}$	1-Pentadecyne	208.37	44	-337.9	2334.5	2334.5	2328.8	44	115-6
	$C_{16}H_{30}$	1-Hexadecyne	222.40	47	-338.1	2490.7	2490.7	2485.0	47	115-6
	$C_{17}H_{32}$	1-Heptadecyne	236.43	50	-338.4	2646.9	2647.0	2641.2	50	115-6
	$C_{18}H_{34}$	1-Octadecyne	250.45	53	-338.6	2803.2	2803.2	2797.5	53	115-6
	$C_{19}H_{36}$	1-Nonadecyne	264.48	56	-338.8	2959.4	2959.5	2953.7	56	115-6
	$C_{20}H_{38}$	1-Eicosyne	278.50	59	-339.0	3115.6	3115.7	3109.9	59	115-6
		$y' = 37.32 + 52.08x'$						$\Sigma x' = 603.0$ $\Sigma y' = 32{,}075.4$ $\Sigma x'y' = 1{,}301{,}601.9$ $\Sigma x'^2 = 24{,}561.0$ $n = 18$		
	C_2H_2	Acetylene	26.04	5	-307.2	-	303.4	-	-	-

*Calculated from gaseous state given in reference 115 by subtracting 86.3 cal/g as in Table 63.

TABLE 76

NORMAL ALKYLBENZENES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^v, KCAL/MOLE OBSERVED	Q_c^v, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_7H_8	Toluene	92.13	18	-312.6	934.5	934.3	926.8	18	115-7
	C_8H_{10}	Ethylbenzene	106.16	21	-316.5	1091.0	1090.7	1085.3	21	115-7
	C_9H_{12}	n-Propylbenzene	120.19	24	-319.5	1247.2	1247.1	1241.5	24	115-7
	$C_{10}H_{14}$	n-Butylbenzene	134.21	27	-321.9	1403.4	1404.0	1397.7	27	115-7
	$C_{11}H_{16}$	n-Amylbenzene	148.24	30	-323.8	1559.[illegible]	1560.1	1554.2	30	115-7
	$C_{12}H_{18}$	n-Hexylbenzene	162.26	33	-325.4	1715.4*	1716.5	1710.7	33	115-7
	$C_{13}H_{20}$	n-Heptylbenzene	176.29	36	-326.7	1872.9*	1873.0	1867.2	36	115-7
	$C_{14}H_{22}$	n-Octylbenzene	190.32	39	-327.9	2029.3*	2029.4	2023.6	39	115-7
	$C_{15}H_{24}$	n-Nonylbenzene	204.34	42	-328.9	2185.6*	2185.9	2180.1	42	115-7
	$C_{16}H_{26}$	n-Decylbenzene	218.37	45	-329.7	2342.3*	2342.3	2336.6	45	115-7
	$C_{17}H_{28}$	n-Undecylbenzene	232.39	48	-330.5	2498.7*	2498.8	2493.0	48	115-7
	$C_{18}H_{30}$	n-Dodecylbenzene	246.42	51	-331.1	2655.2*	2655.2	2649.5	51	115-7
	$C_{19}H_{32}$	n-Tridecylbenzene	260.45	54	-331.7	2811.7*	2811.7	2806.0	54	115-7
	$C_{20}H_{34}$	n-Tetradecylbenzene	274.47	57	-332.2	2968.1*	2968.1	2962.4	57	115-7
	$C_{21}H_{36}$	n-Pentadecylbenzene	288.50	60	-332.8	3124.6*	3124.[illegible]	3118.9	60	115-7
	$C_{22}H_{38}$	n-Hexadecylbenzene	302.52	63	-333.2	3281.1*	3281.0	3275.4	63	115-7
		$y' = -10.14 + 52.15x'$								
								$\Sigma x' = 648.0$ $\Sigma y' = 33,630.7$ $\Sigma x'y' = 1,521,627.0$ $\Sigma x'^2 = 29,304.0$ $n = 16$		
	C_6H_6	Benzene	78.11	15	-307.3	781.0	777.6			115-7
	$C_{13}H_{12}$	Diphenylmethane	168.23	32	-304.3	1653.2	1654.2			88
	$C_{14}H_{14}$	1,1-Diphenylethane	182.25	35	-307.3	1806.1	1810.7			27
	$C_{15}H_{16}$	1,1-Diphenylpropane	196.28	38	-309.8	[illegible]	1967.1			154
	"	1,1-Diphenylpropane	"	"	"	1970.7	"			154
	$C_{16}H_{18}$	1,1-Diphenylbutane	210.30	41	-311.9	2127.6	2123.6			154

*Calculated by subtracting heat of vaporization from gas values given in reference 115 as in Table 77.

TABLE 77

NORMAL ALKYLBENZENES (gas)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^v, KCAL/MOLE OBSERVED	Q_c^v, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_{11}H_{16}$	n-Amylbenzene	148.24	30	-323.5	1574.[illegible]	1572.9	1567.38	30	115-7
	$C_{12}H_{18}$	n-Hexylbenzene	162.26	33	-325.4	1730.33	1730.3	1724.83	33	115-7
	$C_{13}H_{20}$	n-Heptylbenzene	176.29	36	-326.7	1887.77	1887.8	1882.27	36	115-7
	$C_{14}H_{22}$	n-Octylbenzene	190.32	39	-327.9	2045.21	2045.2	2039.71	39	115-7
	$C_{15}H_{24}$	n-Nonylbenzene	204.34	42	-328.9	2202.66	2202.7	2197.16	42	115-7
	$C_{16}H_{26}$	n-Decylbenzene	218.37	45	-329.7	2360.10	2360.1	2354.60	45	115-7
	$C_{17}H_{28}$	n-Undecylbenzene	232.39	48	-330.5	2517.54	2517.5	2512.04	48	115-7
	$C_{18}H_{30}$	n-Dodecylbenzene	246.42	51	-331.1	2674.98	2674.9	2669.48	51	115-7
	$C_{19}H_{32}$	n-Tridecylbenzene	260.45	54	-331.7	2832.43	2832.4	2826.93	54	115-7
	$C_{20}H_{34}$	n-Tetradecylbenzene	274.47	57	-332.3	2989.87	2989.9	2984.37	57	115-7
	$C_{21}H_{36}$	n-Pentadecylbenzene	288.50	60	-332.8	3147.31	3147.3	3141.81	60	115-7
	$C_{22}H_{38}$	n-Hexadecylbenzene	302.52	63	-333.2	3304.76	3304.7	3299.26	63	115-7
		$y' = -7.04 + 52.48x'$								
								$\Sigma x' = 558.0$ $\Sigma y' = 29,199.84$ $\Sigma x'y' = 1,425,335.61$ $\Sigma x'^2 = 27,234.0$ $n = 12$		
	C_6H_6	Benzene	78.11	15	-307.3	789.08	785.7			115-7
	C_7H_8	Toluene	92.13	18	-312.6	943.58	943.1			115-7
	C_8H_{10}	Ethylbenzene	106.16	21	-316.5	1101.13	1101.5			115-7
	C_9H_{12}	n-Propylbenzene	120.19	24	-319.5	1258.24	1258.0			115-7
	$C_{10}H_{14}$	n-Butylbenzene	134.21	27	-323.9	1415.64	1415.5			115-7

TABLE 75

NORMAL ALKYLBENZENES - HEAT OF VAPORIZATION

ADL NO.	FORMULA	NAME	MOL WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_v^o, KCAL/MOLE OBSERVED	Q_v^o, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_6H_6	Benzene		15		8.102	8.118			115-7
	C_7H_8	Toluene		18		9.033	9.090			115-7
	C_8H_{10}	Ethylbenzene		21		10.097	10.062			115-7
	C_9H_{12}	n-Propylbenzene		24		11.053	11.034			115-7
	$C_{10}H_{14}$	n-Butylbenzene		27		11.[illegible]	12.006			115-7
		$y = 3.258 + 0.324x$				$\Sigma x = 105.0$ $\Sigma y = 50.310$ $\Sigma xy = 1065.6230$ $\Sigma x^2 = 2295.00$ $n = 5$				
	$C_{11}H_{16}$	n-Amylbenzene		30		-	12.978			115-7
	$C_{12}H_{18}$	n-Hexylbenzene		33		-	13.950			115-7
	$C_{13}H_{20}$	n-Heptylbenzene		36		-	14.922			115-7
	$C_{14}H_{22}$	n-Octylbenzene		39		-	15.894			115-7
	$C_{15}H_{24}$	n-Nonylbenzene		42		-	16.866			115-7
	$C_{16}H_{26}$	n-Decylbenzene		45		-	17.838			115-7
	$C_{17}H_{28}$	n-Undecylbenzene		48		-	18.810			115-7
	$C_{18}H_{30}$	n-Dodecylbenzene		51		-	19.782			115-7
	$C_{19}H_{32}$	n-Tridecylbenzene		54		-	20.754			115-7
	$C_{20}H_{34}$	n-Tetradecylbenzene		57		-	21.726			115-7
	$C_{21}H_{36}$	n-Pentadecylbenzene		60		-	22.698			115-7
	$C_{22}H_{38}$	n-Hexadecylbenzene		63		-	23.670			115-7

TABLE 77

BRANCHED ALKYLBENZENES (liquid and solid)

ADL NO.	FORMULA	NAME		MOL WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	Q_c^o, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_8H_{10}	o-Xylene	(l)	106.16	21	-316.5	10[illegible].2	10[illegible].7			115-8
	"	m-Xylene	(l)	"	"	"	1037.7	"			115-8
	"	p-Xylene	(l)	"	"	"	1033.7	"			115-8
	C_9H_{12}	Mesitylene	(l)	120.19	24	-319.[illegible]	1241.6	12[illegible].6			115-8
	"	i-Propylbenzene	(l)	"	"	"	124[illegible]	"			115-8
	"	1-Methyl-2-ethylbenzene	(l)	"	"	"	124[illegible].3	"			115-8
	"	1-Methyl-3-ethylbenzene	(l)	"	"	"	124[illegible].7	"			115-8
	"	1-Methyl-4-ethylbenzene	(l)	"	"	"	124[illegible]	"			115-8
	"	1,2,3-Trimethylbenzene	(l)	"	"	"	1242.[illegible]	"			115-8
	"	1,2,4-Trimethylbenzene	(l)	"	"	"	[illegible]	"			115-8
	"	1,3,5-Trimethylbenzene	(l)		"	"	1241.2	"			115-8
	$C_{10}H_{14}$	t-Butylbenzene	(l)	134.21	27	-321.9	14[illegible]	14[illegible].3			115-8
	"	1,2,3,5-Tetramethylbenzene (isodurene)	(l)	"	"	"	1397.[illegible]	"			11
	"	1,2,4,5-Tetramethylbenzene (durene)	(s)	"	"	"	1335.3	"			11
	"	1,2,3,4-Tetramethylbenzene (prehnitene)	(l)	"	"	"	1372.8	"			11
	"	3-n-Propyltoluene	(l)	"	"	"	14[illegible]	"			115-8
	"	3-i-Propyltoluene	(l)	"	"	"	14[illegible]	"			115-8
	"	4-i-Propyltoluene	(l)	"	"	"	14[illegible]	"			115-8
	$C_{11}H_{16}$	Pentamethylbenzene	(s)	148.25	30	-323.[illegible]	1548.7	1559.1			88
	$C_{12}H_{18}$	Hexamethylbenzene	(s)	162.26	33	-32[illegible]	17[illegible]	17[illegible].8			88
		$y = -5.2 + 52.2[illegible]x$ (From n-alkylbenzenes + branched paraffins)									

TABLE 60

POLYBENZENES (solid)

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
		Diphenyls								
	$C_{14}H_{14}$	1,2-Diphenylethane	182.25	35	-307.3	1822.5	1811.2	899.9	17.50	88
	$C_{16}H_{18}$	1,4-Diphenylbutane	210.30	41	-311.9	2127.6	2120.4	1061.3	20.50	154
		Triphenyls								
	$C_{19}H_{16}$	Triphenylmethane	244.32	45	-301.2	2372.7	2372.5	78[illegible].9	15.33	88
	$C_{20}H_{18}$	1,1,1-Triphenylethane	258.34	47	-303.5	2532.4	2530.1	802.2	15.33	27
	"	1,1,2-Triphenylethane	"	"	"	2526.5	"	843.1	16.33	27
		Tetraphenyls								
	$C_{24}H_{18}$	Triphenylbenzene	306.38	57	-297.7	2921.5	2933.8	729.7	14.27	107
	$C_{25}H_{20}$	Tetraphenylmethane	320.41	60	-299.6	3092.3	3091.4	771.7	15.00	27
	$C_{26}H_{22}$	1,1,1,2-Tetraphenylethane	334.44	63	-301.4	3252.3	3247.0	811.7	15.75	27
	"	1,1,2,2-Tetraphenylethane	"	"	"	3248.2	"	810.6	15.75	27
		Pentaphenyls								
	$C_{32}H_{26}$	1,1,1,2,2-Pentaphenylethane	410.53	77	-300.1	3987.4	3967.9	796.3	15.40	27
		$y' = -16.52 + 52.53x'$						$\Sigma x' = 162.14$; $\Sigma y' = 8,352.0$; $\Sigma x'y' = 116,850.983$; $\Sigma x'^2 = 2,655.1942$; $n = 10$		
	$C_{26}H_{22}$	1,1,1,2-Tetraphenylethane	334.44	63	-301.4	3181	3247.0	-	-	152

TABLE 61

BIPHENYLS (liquid)

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	$C_{13}H_{12}$	2-Methylbiphenyl	168.23	32	-304.3	1657.5	1652.5	1654.2	32	18
	"	3-Methylbiphenyl	"	"	"	1654.4	"	1648.7	32	18
	"	4-Methylbiphenyl	"	"	"	1647.2	"	1641.5	32	18
	$C_{14}H_{14}$	3,3'-Dimethylbiphenyl	182.25	35	-307.3	1801.2	1810.4	1795.5	35	18
	"	2-Ethylbiphenyl	"	"	"	1812.5	"	1806.9	35	154
	$C_{15}H_{16}$	2-n-Propylbiphenyl	196.28	38	-309.8	1970.7	1967.5	1955.0	38	154
		$y' = -33.30 + 52.45x'$						$\Sigma x' = 204$; $\Sigma y' = 10,511.8$; $\Sigma x'y' = 358,974.8$; $\Sigma x'^2 = 5966.0$; $n = 6$		
	$C_{12}H_{10}$	Biphenyl (s)	154.20	29	-300.9	1655.0	1657.6			18
	$C_{14}H_{14}$	4,4'-Dimethylbiphenyl (s)	182.25	35	-307.3	1799.3	1810.1			18

TABLE 82

NAPHTHALENES (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	$C_{10}H_8O$	1-Naphthol	144.16	23.0	-27[illegible]	1187.8	1184.7	1181.8	23.0	66
	″	″	″	″	″	1185.4	″	1179.4	23.0	55-225
	″	2-Naphthol	″	″	″	1184.9	″	1178.9	23.0	66
	″	″	″	″	″	1187.2	″	1181.2	23.0	55-225
	$C_{10}H_8$	Naphthalene	128.16	24.0	-299.6	1233.3	1235.4	1227.6	24.0	41
	″	″	″	″	″	1234.5	″	1228.8	24.0	76
	″	″	″	″	″	1232.1	″	1226.4	24.0	13
	″	″	″	″	″	1232.5	″	1226.3	24.0	55-80
	″	″	″	″	″	1231.[illegible]	″	1226.1	24.0	55-52
	″	″	″	″	″	1229.9	″	1224.2	24.0	55-221
	$C_{11}H_8O_2$	2-Naphthoic acid	172.17	″	-223.0	1231.8	1232.4	1229.1	24.0	55-190
	″	″-Naphthoic acid	″	″	″	1227.5	″	1228.9	24.0	55-187
	$C_{10}H_9N$	″-Naphthylamine	143.18	24.5	-273.8	1263.5	1260.0	1256.9	24.5	55-99
	″	″-Naphthylamine	″	″	″	1261.0	″	1255.4	24.5	55-99
	″	″	″	″	″	1260.4	″	1255.3	24.5	153
	$C_{10}H_{10}N_2O_3$	2-Naphthylamine nitrate	206.20	″	-190.1	1260.7	1238.7	1257.4	24.5	153
	$C_{11}H_7N$	1-Naphthonitrile	153.17	25.5	-266.4	1326.2	1321.6	1311.5	25.5	55-102
	″	2-Naphthonitrile	″	″	″	1323.0	″	1309.3	25.5	55-102
	$C_{11}H_{10}$	2-Methylnaphthalene	142.19	27.0	-303.8	1381.9	1387.9	1376.2	27.0	107
	$C_{12}H_{10}O_2$	1-Naphthyl acetate	186.20	″	-232.0	1392.1	1394.7	1371.6	27.0	66
	″	2-Naphthyl acetate	″	″	″	1398.5	″	1388.0	27.0	66
	$C_{16}H_{13}N$	N-Phenyl-2-naphthylamine	219.27	38.5	-280.[illegible]	1987.1	1988.3	1975.1	38.5	111
		$y' = -6.08 + 51.49x'$						$\Sigma x' = 552.5$; $\Sigma y' = 28,314.4$; $\Sigma x'y' = 722,377.5$; $\Sigma x'^2 = 14,052.75$; $n = 22$		
	$C_{12}H_8O_4$	1,8-Naphthalenedicarboxylic acid	216.18	24.0	-177.6	1240.1	1227.7			55-127
	$C_{17}H_{12}O_2$	2-Naphthyl benzoate	248.27	38.0	-244.9	1966.0	1958.9			7
	$C_{21}H_{16}O_2$	2-Naphtholformal	300.34	48.0	-255.7	2500.5	2507.9			55-60

TABLE 83

PRIMARY ALCOHOLS (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	CH_4O	Methyl alcohol	32.04	3	-149.8	173.6	170.9	167.9	3	113
	C_2H_6O	Ethyl alcohol	46.07	6	-208.4	326.7	326.9	321.0	6	113
	C_3H_8O	n-Propyl alcohol	60.09	9	-239.6	482.2	483.0	476.5	9	113
	$C_4H_{10}O$	n-Butyl alcohol	74.12	12	-259.0	638.1	639.2	632.4	12	113
	$C_5H_{12}O$	n-Amyl alcohol	88.15	15	-272.3	794.[illegible]	795.[illegible]	788.6	15	113
	$C_6H_{14}O$	n-Hexyl alcohol	102.17	18	-281.9	950.6	951.3	944.9	18	113
	$C_7H_{16}O$	n-Heptyl alcohol	116.20	21	-289.2	1107.1	1107.4	1101.4	21	113
	$C_8H_{18}O$	n-Octyl alcohol	130.22	24	-294.9	1263.6	1263.5	1257.9	24	113
	$C_9H_{20}O$	n-Nonyl alcohol	144.25	27	-299.5	1420.2	1419.6	1414.[illegible]	27	113
	$C_{10}H_{22}O$	n-Decyl alcohol	158.28	30	-303.3	1576.9	1575.7	1571.2	30	113
		$y' = 9.17 + 52.03x'$						$\Sigma x' = 165.0$; $\Sigma y' = 8676.3$; $\Sigma x'y' = 181,790.7$; $\Sigma x'^2 = 3465.0$; $n = 10$		

TABLE 64

PRIMARY ALCOHOLS (gas)

ADL NO	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	Q_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	CH_4O	Methyl alcohol	32.04	3	-149.8	182.58	180.5	177.08	3	113
	C_2H_6O	Ethyl alcohol	46.07	6	-208.4	336.78	337.2	331.28	6	113
	C_3H_8O	n-Propyl alcohol	60.09	9	-239.6	493.20	493.9	487.70	9	113
	$C_4H_{10}O$	n-Butyl alcohol	74.12	12	-259.0	649.90	650.6	644.40	12	113
	$C_5H_{12}O$	n-Amyl alcohol	88.15	15	-272.3	806.75	807.4	801.25	15	113
	$C_6H_{14}O$	n-Hexyl alcohol	102.17	18	-281.9	963.60	964.1	958.10	18	113
	$C_7H_{16}O$	n-Heptyl alcohol	116.20	21	-289.2	1120.60	1120.8	1115.10	21	113
	$C_8H_{18}O$	n-Octyl alcohol	130.22	24	-294.9	1277.70	1277.5	1272.10	24	113
	$C_9H_{20}O$	n-Nonyl alcohol	144.25	27	-299.5	1434.60	1434.2	1429.10	27	113
	$C_{10}H_{22}O$	n-Decyl alcohol	158.28	30	-303.3	1591.60	1591.0	1586.10	30	113
		$y' = 18.26 + 52.2[illegible]x'$								

$\Sigma x' = 165.0$
$\Sigma y' = 8602.21$
$\Sigma x'y' = 164,021.77$
$\Sigma x'^2 = 3465.0$
$n = 10$

TABLE 65

SECONDARY ALCOHOLS (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	Q_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_3H_8O	1-Propyl alcohol	60.09	9	-239.6	474.8	473.0	469.1	9	67
	$C_6H_{12}O$	Cyclohexanol	100.16	17	-271.6	890.7	885.5	892.4	17	55-153
	"	2-Methylcyclopentanol	"	"	"	887.4	"	883.5	17	55-215
	$C_6H_{14}O$	Pinacolyl alcohol	102.17	18	-281.9	935.6	939.7	932.9	18	55-215
	$C_7H_{14}O$	3-Methylcyclohexanol	114.18	20	-280.3	1035.4	1042.4	1040.1	20	55-215
	"	1-Ethyl-2-cyclopentanol	"	"	"	1039.0	"	1034.9	20	55-215
	"	1,3-Dimethyl-2-cyclopentanol	"	"	"	1030.5	"	1025.4	20	55-215
	$C_8H_{16}O$	1,3-Dimethyl-2-cyclohexanol	128.21	23	-287.0	1196.0	1190.5	1197.7	23	55-215
	"	1,3-Dimethyl-5-cyclohexanol	"	"	"	1183.4	"	1185.3	23	55-215
	$C_{14}H_{18}O$	1-Phenyl-2-octyne-1-ol (Amylphenylpropargyl alcohol)	202.29	36	-284.8	1901.1	1899.0	1865.7	36	55-138
		$y' = 4.57 + 51.64x'$								

$\Sigma x' = 203.0$
$\Sigma y' = 10,528.0$
$\Sigma x'y' = 235,206.6$
$\Sigma x'^2 = 4537.0$
$n = 10$

TABLE 66

TERTIARY ALCOHOLS (liquid)

ADL NO	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	Q_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_4H_{10}O$	t-Butyl alcohol	74.12	12	-259.0	629.3	627.7	621.6	12	55-215
	$C_5H_{12}O$	Dimethyl ethyl carbinol	88.15	15	-272.3	784.6	781.3	773.9	15	55-215
	$C_6H_{12}O$	Allyl dimethyl carbinol	100.16	17	-271.6	900.1	897.9	880.5	17	55-215
	$C_6H_{14}O$	Methyl diethyl carbinol	102.17	18	-281.9	927.0	934.6	921.3	18	55-215
	$C_7H_{16}O$	Triethyl carbinol	116.20	21	-289.2	1080.0	1088.0	1074.3	21	55-215
	$C_8H_{18}O$	Methyl dipropyl carbinol	130.22	24	[illegible]	1232.7	1241.4	1227.0	24	55-215
	$C_9H_{20}O$	Ethyl dipropyl carbinol	144.25	27	-299.5	1386.5	1394.8	1380.8	27	55-215
	$C_7H_{14}O$	1,3-Dimethyl-3-cyclopentanol	114.18	20	-280.3	1034.0	1035.3	1029.9	20	55-215
	"	Allyl methyl ethyl carbinol	"	"	"	1050.1	1050.7	1030.4	20	55-215
	$C_8H_{16}O$	1,2-Dimethyl-2-cyclohexanol	128.21	23	-287.0	1176.5	1182.9	1193.2	23	55-163
	"	1,3-Dimethyl-3-cyclohexanol	"	"	"	1192.5	"	1194.2	23	55-215
	"	Allyl methyl propyl carbinol	"	"	"	1201.9	1204.3	1182.2	23	55-215
	"	Allyl diethyl carbinol	"	"	"	1207.1	"	1187.4	23	55-215
	$C_9H_{18}O$	1-Methyl-3-ethylcyclohexanol-3	142.23	26	-292.5	1322.4	1336.3	1324.1	26	55-215
	"	Allyl [illegible] n-butyl carbinol	"	"	"	1341.3	1357.6	1346.1	26	55-215
	"	Allyl methyl t-butyl carbinol	"	"	"	1363.0	"	1343.4	26	55-215
	$C_{10}H_{18}O$	Diallyl propyl carbinol	154.24	28	-270.5	1472.1	1468.3	1444.0	28	55-215
	$C_{11}H_{22}O$	Allyl methyl hexyl carbinol	170.29	32	-300.7	1666.7	1664.4	164[illegible].1	32	55-215
		$y' = 7.54 + 51.13x'$								

$\Sigma x' = 404.0$
$\Sigma y' = 20,812.1$
$\Sigma x'y' = 495,206.00$
$\Sigma x'^2 = 9460.0$
$n = 18$

TABLE 87

MIXED POLYALCOHOLS (liquid)

AD. NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	$C_2H_6O_2$	Ethylene glycol	62.07	5	-128.9	284.3	283.5	139.2	2.50	88
	$C_3H_8O_2$	1,2-Propanediol	76.09	8	-168.2	436.7	437.8	225.5	4.00	82
	$C_4H_{10}O_2$	1,2-Butanediol	90.12	11	-195.3	593.8	592.2	294.1	5.50	82
	"	1,3-Butanediol	"	"	"	595.8	"	[illegible]	5.50	82
	"	2,3-Butanediol	"	"	"	589.5	"	291.9	5.50	82
	"	2-Methyl-1,2-propanediol	"	"	"	589.9	"	292.1	5.50	82
	$C_3H_8O_3$	Glycerol	92.09	7	-121.6	395.6	396.7	130.0	2.33	88

$y' = 10.26 + 51.45x'$ for a single OH

$\Sigma x' = 30.83$
$\Sigma y' = 1,658.0$
$\Sigma x'y' = 7,965.750$
$\Sigma x'^2 = 149.6789$
$n = 7$

TABLE 88

MIXED POLYALCOHOLS (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	$C_5H_{12}O_4$	Pentaerythritol	136.15	12	-141.0	661.2	661.1	163.9	3.00	55-195
	$C_4H_{10}O_4$	Erythritol	122.12	9	-117.9	500.2	501.1	123.6	2.25	88
	$C_5H_{12}O_5$	Arabitol	152.15	11	-115.7	611.8	611.6	121.2	2.20	55-195
	$C_6H_{14}O_6$	Dulcitol	182.17	13	-114.2	720.6	722.1	119.2	2.17	88
	"	Mannitol	"	"	"	722.5	"	119.5	2.17	88
	$C_7H_{16}O_7$	Glucoheptitol	212.20	15	-113.1	835.8	832.6	118.6	2.14	55-195

$y' = 3.8 + 53.35x'$ for a single OH

$\Sigma x' = 13.93$
$\Sigma y' = 766.0$
$\Sigma x'y' = 1,802.723$
$\Sigma x'^2 = 32.2499$
$n = 6$

TABLE 89

AROMATIC HYDROXYLS (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	C_6H_6O	Phenol	94.11	14	-238.0	730.6	726.7	734.0	14.0	9
	$C_7H_8O_2$	o-Hydroxybenzyl alcohol	124.13	16	-206.2	845.4	840.7	840.3	16.0	55-44
	C_7H_8O	m-Cresol	108.13	17	-251.5	883.5	884.2	885.7	17.0	9
	"	p- "	"	"	"	885.0	"	888.2	17.0	12
	"	o- "	"	"	"	883.7	"	885.9	17.0	12
	$C_8H_{10}O$	o-Xylenol	122.16	20	-262.0	1035.1	1037.9	1040.0	20.0	55-201
	"	m- "	"	"	"	1037.4	"	1042.1	20.0	55-201
	"	p- "	"	"	"	1035.[illegible]	"	1040.2	20.0	55-201
	$C_9H_{12}O$	Pseudocumenol	136.19	23	-270.2	1191.8	[illegible]	[illegible]	23.0	55-201
	$C_{10}H_8O$	1-Naphthol	144.16	23	-255.3	1185.4	1185.6	1198.0	23.0	55-225
	"	1- "	"	"	"	1187.5	"	1200.4	23.0	66
	"	2- "	"	"	"	1187.2	"	1199.8	23.0	55-225
	"	2- "	"	"	"	1184.9	"	1197.5	23.0	66
	$C_{10}H_{14}O$	Thymol	150.21	26	-276.9	1353.7	1349.6	1353.6	26.0	55-201
	$C_6H_6O_2$	Pyrocatechol	110.11	13	-188.9	684.8	685.7	344.2	6.5	55-195
	"	Resorcinol	"	"	"	683.0	"	343.3	6.5	55-195
	"	Hydroquinone	"	"	"	683.2	"	343.4	6.5	55-225
	$C_7H_8O_2$	Toluhydroquinone	124.13	16	-206.2	835.1	839.3	419.2	8.0	55-225
	$C_{10}H_{14}O_2$	Thymohydroquinone	166.21	25	-240.7	1307.1	1304.7	655.6	12.5	55-225
	$C_{15}H_{16}O_2$	p,p'-1-Propylidenediphenol	228.29	36	-252.3	1844.1	1846.0	940.8	18.0	45
	$C_{21}H_{16}O_2$	1,1'-Methylenedi(2-naphthol)	300.34	48	-255.7	2475.8	2467.6	1254.1	24.0	55-60
	$C_6H_6O_3$	Pyrogallol	126.11	12	-152.2	638.7	639.[illegible]	214.1	4.0	55-195
	$C_{12}H_{10}O$	2-Phenylphenol	170.20	28	-263.2	1482.5	1483.[illegible]	-	-	14

$y' = [illegible] + 51.79x'$

$\Sigma x' = 366.0$
$\Sigma y' = 19,212.5$
$\Sigma x'y' = 37[illegible]39.55$
$\Sigma x'^2 = [illegible]$
$n = 22$

TABLE 90

ETHERS (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	$C_3H_8O_2$	2-Methoxyethanol	76.09	8.0	-168.2	441.2	447.6	436.7	8.0	125
	$C_4H_{10}O_3$	Diethylene glycol	106.12	10.0	-150.8	555.7	561.0	545.2	10.0	82
	$C_4H_{10}O$	Diethyl ether	74.12	12.0	-259.0	651.7	647.6	654.0	12.0	55-204
	C_7H_8O	Anisole	108.13	17.0	-251.5	903.9	899.7	907.1	17.0	9
	$C_8H_{10}O$	Phenetole	122.16	20.0	-262.0	1056.5	1056.5	1059.6	20.0	9
	"	m-Cresol methyl ether	"	"	"	1057.5	"	1060.6	20.0	9
	$C_9H_{12}O$	m-Xylenol methyl ether	136.19	23.0	-270.2	1213.4	1211.7	1217.8	23.0	55-203
	"	p-Cresol ethyl ether	"	"	"	1212.8	1213.3	1215.6	23.0	55-203
	"	Phenyl propyl ether	"	"	"	1213.1	"	1315.9	23.0	55-203
	$C_{10}H_{14}O$	p-Xylenol ethyl ether	150.21	26.0	-276.9	1368.5	1368.5	1372.5	26.0	55-203
	$C_{11}H_{16}O$	Thymol methyl ether	164.24	29.0	-282.5	1524.3	1525.8	1527.8	29.0	55-203
	$C_{12}H_{18}O$	Thymol ethyl ether	178.26	32.0	-287.2	1679.9	1682.9	1682.9	32.0	55-203
	$C_5H_{12}O_3$	Diethylene glycol monomethyl ether	120.15	13.0	-173.1	720.2	721.8	353.0	6.5	125
	$C_6H_{14}O_4$	Triethylene glycol	150.17	15.5	-164.0	857.8	857.5	440.2	7.75	82
	$C_6H_{14}O_2$	Glycol diethyl ether	118.17	17.0	-230.2	[illegible]	922.1	437.5	8.5	55-172
	$C_8H_{18}O_5$	Tetraethylene glycol	196.24	21.0	-171.2	1116.9	1165.6	374.7	7.0	82
		$y' = 15.47 + 52.20x'$						$\Sigma x' = 272.75$ $\Sigma y' = 14,495.1$ $\Sigma x'y' = 304,299.90$ $\Sigma x'^2 = 5,746.5625$ $n = 16$		
	$C_{10}H_{22}O$	Diamyl ether	158.28	10	-303.3	1603.3	1597.2	-	-	55-65

TABLE 91

ALIPHATIC ETHERS (gas)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	C_2H_6O	Dimethyl ether	46.07	6	-208.4	347.6	348.2	342.1	6	55-223
	C_3H_8O	Methyl ethyl ether	60.09	9	-239.6	501.4	495.5	497.9	9	55-223
	C_4H_6O	Methyl propargyl ether	70.09	10	-228.3	600.8	595.2	558.0	10	55-223
	C_4H_8O	Methyl allyl ether	72.10	11	-244.1	623.9	624.5	604.3	11	55-223
	$C_4H_{10}O$	Diethyl ether	74.12	12	-259.0	660.3	662.8	654.[illegible]	12	55-204
	$C_6H_{10}O$	Diallyl ether	98.14	16	-260.9	906.6	906.8	867.[illegible]	16	55-223
		$y' = 28.1 + 52.43x'$						$\Sigma x' = 64.0$ $\Sigma y' = 3524.3$ $\Sigma x'y' = 40,493.8$ $\Sigma x'^2 = 739.0$ $n = 6$		

TABLE 92

OXIRANES (Ethylene Oxide) (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF
	C_2H_4O	Ethylene oxide	44.05	5	-181.6	302.4	302.1	296.7	5	82
	C_3H_6O	1,2-Propylene oxide	58.08	8	-220.4	455.4	455.3	447.7	8	82
	C_4H_8O	1,2-Butene oxide	72.10	11	-244.1	610.2	606.2	604.5	11	82
	$C_6H_{12}O$	3,4-Hexene oxide	100.16	17	-2[illegible].6	913.9	914.4	902.2	17	55-245
		$y' = 41.2 + 51.03x'$						$\Sigma x' = 41$ $\Sigma y' = 2257.1$ $\Sigma x'y' = 27,154.0$ $\Sigma x'^2 = 499.0$ $n = 4$		
	$C_5H_{10}O$	2-Methyl-2,3-butene oxide	86.13	14	-260.1	749.8	761.3	-	-	55-245

[illegible]

[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

[illegible]

[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

TABLE [illegible]

[illegible] (Liquid)

Formula	Name	Mol. Wt.	Oxygen	Oxygen Balance	Q^{c}, kcal/mole Observed	Q^{c}, kcal/mole Calculated	Y	X'	Ref.
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	625.3	621.0	[illegible]	73
[illegible]	[illegible]	72.1[illegible]	11	[illegible]	587.3	587.9	576.6	11	37
[illegible]	[illegible]	[illegible]	6	900.2	737.0	737.7	727.5	14	55-215
	[illegible]				733.6		739.2	14	55-215
[illegible]	[illegible]	[illegible]	17	[illegible]	865.2	[illegible]	[illegible]	17	55-215
[illegible]	[illegible]	[illegible]	22	[illegible]	[illegible]	1010.9	1022.6	20	55-215
	[illegible]				1045.5	1047.1	1041.7	[illegible]	55-215
[illegible]	[illegible]	131.31	23	[illegible]	1244.1	1256.7	[illegible]	23	55-215

[illegible] 8.47 [illegible] 51.84

$\Sigma x' = 12[illegible]$
$\Sigma y' = 663[illegible].8$
$\Sigma x'y' = 114,59[illegible]$
$\Sigma x'^2 = 2195.0$
$n = 8$

TABLE [illegible]7

[illegible] (Liquid)

Formula	Name	Mol. Wt.	Oxygen per 100	Oxygen Balance	Q^{c}, kcal/mole Observed	Q^{c}, kcal/mole Calculated	Y	X'	Ref.
[illegible]	[illegible] acid	[illegible]		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible] acid	74.08	[illegible]	[illegible]	[illegible]	365.1	357.[illegible]	[illegible]	[illegible]
[illegible]	[illegible]butyric acid	88.[illegible]	10	[illegible]	[illegible]	[illegible].5	515.[illegible]	[illegible]	[illegible]
	[illegible]butyric acid				[illegible]	[illegible]	511.[illegible]	[illegible]	[illegible]
[illegible]	[illegible] acid	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	675.[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	226.5	[illegible]	[illegible]
	[illegible] acid				[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	[illegible] acid				[illegible]		[illegible]		[illegible]
[illegible]	[illegible]	[illegible]	19	[illegible]	994.5	[illegible]	[illegible]		[illegible]
	[illegible] acid				994.1	[illegible].9	[illegible]		[illegible]
[illegible]	[illegible] acid	[illegible]	[illegible]	[illegible]	[illegible]	1116.5	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	158.2[illegible]	25	[illegible]	[illegible]	[illegible]	[illegible]292.[illegible]	26	[illegible]

[illegible]

$\Sigma x' = 17[illegible]$
$\Sigma y' = 91[illegible]$
$\Sigma x'y' = 1[illegible]$
$\Sigma x'^2 = [illegible]$
$n = 12$

Formula	Name	Mol. Wt.	Oxygen per 100	Oxygen Balance	Q^{c}, kcal/mole Observed	Q^{c}, kcal/mole Calculated	Y	X'	Ref.
[illegible]	Formic acid	46.03	1	[illegible]	62.9		63.[illegible]		[illegible]

TABLE 98

ACIDS (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	Q_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
		Monocarboxylic								
	$C_{10}H_{20}O_2$	Capric acid	172.26	28	-260.1	1458.1	[illegible]	[illegible]	28	55-192
	$C_{11}H_{22}O_2$	Undecylenic acid	186.29	31	-266.3	1615.9	1616.1	1610.2	31	55-192
	$C_{12}H_{24}O_2$	Lauric acid	200.31	34	-271.6	1774.8	1772.3	1769.1	34	118
	$C_{14}H_{28}O_2$	Myristic acid	228.36	40	-280.3	2085.2	2084.7	2080.1	40	55-193
	$C_{16}H_{32}O_2$	Palmitic acid	256.42	46	-287.0	2391.5	2397.1	2385.8	46	55-192, 55-64 (Av.)
	$C_{18}H_{36}O_2$	Stearic acid	284.4	52	-292.5	2704.8	2709.6	2699.1	52	55-192, 55-64 (Av.)
	$C_{20}H_{40}O_2$	Arachidic acid	312.52	58	-296.9	3025.9	3022.0	3020.2	58	55-192
	$C_{22}H_{44}O_2$	Behenic acid	340.57	64	-300.7	[illegible]	[illegible]	[illegible]	64	55-193
		Dicarboxylic-Straight Chain								
	$C_3H_4O_4$	Malonic acid	104.06	4	- 61.5	206.5	206.5	100.4	2.0	148
	$C_4H_6O_4$	Succinic acid	118.09	7	- 94.8	356.2	362.7	175.3	3.5	47
	$C_5H_8O_4$	Glutaric acid	132.11	10	-121.1	514.9	518.9	254.6	5.0	148
	$C_6H_{10}O_4$	Adipic acid	146.14	13	-142.3	668.9	677.1	331.6	6.5	148
	$C_7H_{12}O_4$	Pimelic acid	160.17	16	-159.8	827.7	831.3	431.0	8.0	148
	$C_8H_{14}O_4$	Suberic acid	174.19	19	-174.5	983.2	987.5	489.8	9.5	148
	$C_9H_{16}O_4$	Azelaic acid	188.2	22	-187.0	1141.7	1143.7	568.3	11.0	148
	$C_{10}H_{18}O_4$	Sebacic acid	202.24	25	-197.8	1297.3	1299.9	645.8	12.5	148
	$C_{11}H_{20}O_4$	Nonanedicarboxylic acid	216.27	28	-207.1	1455.6	1456.1	725.0	14.0	148
	$C_{12}H_{22}O_4$	Decanedicarboxylic acid	230.30	31	-215.4	1610.7	1612.3	802.5	15.5	148
	$C_{13}H_{24}O_4$	Brassylic acid	244.32	34	-222.7	1768.6	1768.5	881.5	17.0	148
		Dicarboxylic-Branched Chain								
	$C_4H_6O_4$	Methylmalonic acid	118.09	7	- 94.8	363.6	359.6	173.5	3.5	55-192
	$C_5H_8O_4$	Ethylmalonic acid	132.11	10	-121.1	519.2	516.1	258.3	5.0	145
	"	Methylsuccinic acid	"	"	"	512.7	"	254.9	5.0	147
	"	Dimethylmalonic acid	"	"	"	515.1	"	[illegible]	[illegible]	55-190
	$C_6H_{10}O_4$	α-Methylglutaric [illegible]	146	13	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

TABLE 99

ACID ANHYDRIDES (liquid)

AUL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^0, KCAL/MOLE OBSERVED	Q_c^0, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_4H_6O_3$	Acetic anhydride	102.09	8	-12[illegible]	431.9	431.3	426.2	8	55-223
	$C_6H_8O_3$	Ethylsuccinic anhydride	128.12	13	-16[illegible]	665.4	669.1	[illegible]2.2	13	147
	$C_6H_{10}O_3$	Propionic anhydride	130.14	14	-172.1	746.6	740.6	740.9	14	55-118

$y' = 7.18 + 52.07x'$

$\Sigma x' = 35.0$
$\Sigma y' = 18[illegible].3$
$\Sigma x'y' = 22,690.60$
$\Sigma x'^2 = 429.0$
$n = 3$

TABLE 100

ACID ANHYDRIDES (solid)

AUL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^0, KCAL/MOLE OBSERVED	Q_c^0, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_4H_4O_3$	Succinic anhydride	100.07	7	-111.9	369.9	372.6	364.2	7	147
	$C_5H_6O_3$	Glutaric anhydride	[illegible]	10	-140.2	525.0	528.6	522.3	10	55-133
	"	Methylsuccinic anhydride		"		52[illegible].2	52[illegible]	525.3	10	147
	$C_6H_8O_3$	asym-Dimethylsuccinic anhydride	128.12	13	-162.3	683.3	682.5	680.1	13	147
	"	cis-sym-Dimethylsuccinic anhydride	"	"	"	681.7	"	678.5	13	147
	"	trans-sym-Dimethylsuccinic anhydride	"	"	"	677.9	"	676.7	13	147
	$C_7H_{10}O_3$	Trimethylsuccinic anhydride	142.15	16	-180.[illegible]	837.0	838.9	833.6	16	147
	$C_8H_{12}O_3$	Tetramethylsuccinic anhydride	156.18	19	-194.6	993.7	995.4	990.0	19	147
	"	asym-Diethylsuccinic anhydride	"	"	"	997.5	"	995.8	19	147
	"	cis-sym-Diethylsuccinic anhydride	"	"	"	99[illegible].4	"	994.7	19	147
	"	trans-sym-Diethylsuccinic anhydride	"	"	"	996.8	"	993.1	19	147
	$C_{10}H_{16}O_3$	Triethylsuccinic anhydride	184.23	25	-217.1	1311.2	1304.4	1307.0	25	147
	$C_{12}H_{20}O_3$	Tetraethylsuccinic anhydride	212.28	31	-233.7	1623.5	1621.4	1620.7	31	147
	$C_{14}H_{26}O_3$	Diisoamylacetic anhydride	214.30	32	-238.9	1660.3	1673.5	1664.2	32	55-227
	$C_{14}H_{26}O_3$	Heptylic anhydride	242.35	35	-250.4	1985.5	1936.0	19[illegible]	35	55-227

$y' = 2.62 + 52.07x'$

$\Sigma x' = 236.[illegible]$
$\Sigma y' = 14,824.0$
$\Sigma x'y' = 339,661.8$
$\Sigma x'^2 = 6510.0$
$n = 15.0$

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TABLE 101

ESTERS (liquid)

ADD. NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c, KCAL/MOLE OBSERVED	Q_c, KCAL/MOLE CALCULATED	Y'	X'	REF.
		Of Monocarboxylic Acids								
	$C_2H_4O_2$	Methyl formate	60.05	4	-106.6	[illegible]	[illegible]	227.4	4.0	55-26
	$C_3H_6O_2$	Methyl acetate	74.06	7	-151.2	360.6	381.4	374.9	7.0	123
	"	Ethyl formate	"	"	"	391.7	"	[illegible]	7.0	55-26
	$C_4H_8O_2$	Ethyl acetate	88.10	10	-181.6	535.1	538.4	529.4	10.0	123
		Methyl propionate	"	"	"	536.9	"	531.2	10.0	123
	$C_5H_{10}O_2$	Propyl acetate	102.13	13	-203.7	690.9	693.4	685.2	13.0	123
	"	Ethyl propionate	"	"	"	690.3	"	684.6	13.0	123
	"	Methyl n-butyrate	"	"	"	693.0	"	687.4	13.0	123
	"	i-Propyl acetate	"	"	"	688.2	690.9	685.0	13.0	123
	"	Methyl i-butyrate	"	"	"	694.2	"	691.0	13.0	55-154
	$C_6H_{12}O_2$	Ethyl n-butyrate	116.16	16	-220.4	845.9	841.4	840.2	16.0	123
	"	n-Propyl propionate	"	"	"	847.3	"	841.6	16.0	123
	"	n-Butyl acetate	"	"	"	846.7	"	841.0	16.0	123
	"	i-Butyl acetate	"	"	"	844.7	846.1	841.3	16.0	123
	"	i-Propyl propionate	"	"	"	844.0	"	840.6	16.0	123
	"	Ethyl i-butyrate	"	"	"	845.7	"	842.1	16.0	55-118
	$C_7H_{14}O_2$	n-Butyl propionate	130.18	19	-231.5	[illegible]	1001.3	993.2	19.0	123
	"	n-Propyl n-butyrate	"	"	"	1001.9	"	996.2	19.0	123
	"	Ethyl valerate	"	"	"	1017.5	"	1011.8	19.0	55-65
	"	i-Amyl acetate	"	"	"	[illegible]	1001.3	996.7	19.0	123
	"	i-Butyl propionate	"	"	"	[illegible]	"	996.6	19.0	123
	"	i-Propyl n-butyrate	"	"	"	1000.1	"	996.4	19.0	123
	$C_8H_{16}O_2$	n-Butyl n-butyrate	144.21	22	-244.1	1157.8	1159.3	1152.1	22.0	123
	"	i-Amyl propionate	"	"	"	1156.9	1156.6	1152.9	22.0	123
	"	i-Butyl n-butyrate	"	"	"	1157.1	"	1152.1	22.0	123
	$C_9H_{18}O_2$	i-Amyl n-butyrate	158.23	25	-252.8	1312.4	1311.9	1306.2	25.0	123
		Of Dicarboxylic Acids								
	$C_5H_8O_4$	Dimethyl malonate	132.11	[illegible]	-121.1	554.0	554.4	274.2	5.0	[illegible]
	$C_6H_{10}O_4$	Dimethyl succinate	146.14	13	-142.3	707.1	709.5	350.7	6.5	116
	"	Diethyl oxalate	"	"	"	715.0	"	355.2	6.5	55-119
	$C_7H_{12}O_4$	Dimethyl glutarate	160.17	15	[illegible]	863.2	864.6	428.8	8.0	116
	"	Diethyl malonate	"	"	"	860.4	"	427.4	8.0	55-119
	$C_8H_{14}O_4$	Dimethyl adipate	174.19	19	-174.5	1019.6	1019.5	507.0	9.5	116
	"	Diethyl succinate	"	"	"	1007.3	"	500.8	9.5	55-119
	$C_9H_{16}O_4$	Dimethyl pimelate	188.22	22	-187.0	1176.0	1174.5	585.2	11.0	116
	$C_{10}H_{18}O_4$	Dimethyl suberate	202.24	25	-197.8	1332.3	1329.5	663.3	12.5	116
		Diethyl dimethylsuccinate (sym)	"	"	"	1323.9	1327.8	662.4	12.5	55-131
	"	Diethyl dimethylsuccinate (racemic)	"	"	"	1322.9	[illegible]	659.4	12.5	55-[illegible]
	$C_{11}H_{20}O_4$	Dimethyl azelate	216.27	28	-207.1	1488.3	1484.3	741.3	14.0	116
	$C_{12}H_{22}O_4$	Dimethyl sebacate	230.30	31	-215.4	1644.7	1639.[illegible]	[illegible]	15.5	116

$y' = 16.08 + 51.66x'$

$\Sigma x' = 535.0$
$\Sigma y' = 28,265.[illegible]$
$\Sigma x'y' = 441,661.95$
$\Sigma x'^2 = 8,[illegible]2.0$
$n = 39.0$

TABLE 102

ESTERS (solid)

ADD. NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c, KCAL/MOLE OBSERVED	Q_c, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_4H_6O_4$	Dimethyl oxalate	118.09	7	-94.8	400.8	398.1	197.6	3.5	116
	$C_{10}H_{18}O_4$	Diethyl dimethylsuccinate (meso)	202.24	25	-197.8	1324.1	1323.0	660.0	12.5	55-9[illegible]
	$C_{10}H_{14}O_8$	Tetramethyl ethanetetracarboxylate	262.21	19	-115.9	1045.1	1047.7	459.9	4.75	55-133
	$C_{11}H_{16}O_8$	Tetramethyl methylenedimalonate	276.24	22	-127.4	1201.4	1202.1	[illegible]	[illegible]	55-137
	$C_{14}H_{22}O_8$	Tetraethyl ethanetetracarboxylate	318.32	31	-155.8	1661.2	1665.3	813.9	7.75	55-7

$y' = 16.13 + 51.46x'$

$\Sigma x' = 44.0$
$\Sigma y' = 1830.3$
$\Sigma x'y' = 15,027.8$
$\Sigma x'^2 = 281.375$
$n = 5$

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TABLE 103

NITRILES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	Q_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_2H_3N	Acetonitrile	41.05	5.5	-214.4	302.4	301.1	295.7	5.5	55-102
	C_2H_3NO	Glycolonitrile	57.05	4.5	-126.2	[illegible]	[illegible]	242.0	4.5	55-24
	C_3H_3N	Acrylonitrile	53.06	7.5	-226.2	420.4	419.6	400.6	7.5	32
	C_3H_5N	Propionitrile	55.08	8.5	-246.9	465.4	457.6	450.7	8.5	55-102
	$C_4H_5NO_2$	Methyl cyanoacetate	99.09	"	-137.2	471.6	470.1	453.4	8.5	55-78
	C_4H_5N	Allyl cyanide	67.09	10.5	-250.4	574.9	575.8	555.1	10.5	55-51
	"	Crotonitrile	"	"	"	571.9	"	552.1	10.5	55-51
	C_4H_7N	n-Butyronitrile	69.10	11.5	-266.3	613.3	613.8	607.6	11.5	55-102
	$C_5H_7NO_2$	Ethyl cyanoacetate	113.11	"	-162.7	630.0	625.1	613.0	11.5	55-78
	C_5H_9N	i-Valeronitrile	83.13	14.5	-279.1	772.1	757.6	768.8	14.5	55-102
	$C_8H_{11}N$	Amylpropiolonitrile	121.18	21.5	-283.9	1164.2	1171.8	1121.2	21.5	55-138
	$C_{13}H_9N$	o-Cyanobiphenyl	179.21	30.5	-272.3	1566.3	1583.1	1600.6	30.5	18
	$C_4H_4N_2$	Succinonitrile	80.09	10.0	-199.8	545.7	[illegible]	270.0	5.0	55-41
		$y' = 9.33 + 52.07x'$						$\Sigma x' = 150.0$ $\Sigma y' = 7931.8$ $\Sigma x'y' = 15?,?94.4$ $\Sigma x'^2 = 2364.0$ $n = 13$		
	C_3N_2O	Carbonyl cyanide	80.05	5.0	-99.9	332.0	289.2	-	-	50
	~~C_3H_5NO~~	~~Acetaldehyde cyanohydrin~~	~~71.08~~	~~7.5~~	~~-179.4~~	~~421.1~~	~~405.7~~	-	-	55-24
	$C_6H_9NO_2$	Propyl cyanoacetate	127.14	14.5	-182.5	769.0	780.0	-	-	55-78

TABLE 104

NITRILES (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	Q_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_3H_3NO_2$	Cyanoacetic acid	85.06	5.5	-103.5	293.8	296.3	287.4	5.5	55-78
	$C_3H_4N_2O$	Cyanoacetamide	84.08	7.0	-133.2	376.3	377.7	374.2	7.0	55-78
	$C_6H_7NO_3$	Methyl acetylcyanoacetate	141.12	12.5	-141.7	665.0	683.2	665.3	12.5	55-78
	$C_3H_2N_2$	Malononitrile	66.06	7.0	-169.5	394.8	390.1	194.6	3.5	55-41
	$C_5H_6N_2$	Glutaronitrile	94.12	13.0	-221.0	699.6	708.3	347.9	6.5	55-41
	$C_8H_4N_2$	Phthalonitrile	128.13	18.0	-224.8	955.4	957.3	479.3	9.0	121
		$y' = 6.90 + 52.37x'$						$\Sigma x' = 44.0$ $\Sigma y' = 2357.7$ $\Sigma x'y' = 17,???.??$ $\Sigma x'^2 = 371.0$ $n = 6$		
	C_4N_2	Carbon subnitride	76.06	8.0	-168.3	511.8	[illegible]	-	-	55-139

TABLE 105

CARBYLAMINES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	Q_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_2H_3N	Methyl carbylamine	41.05	5.5	-214.4	317.4	321.9	311.7	5.5	55-93
	"	"	"	"	"	320.1	"	314.4	5.5	55-77
	C_3H_5N	Ethyl carbylamine	55.08	8.5	-246.9	477.1	479.8	471.4	8.5	55-94
	"	"	"	"	"	480.5	"	474.8	8.5	55-77
	C_4H_5N	Allyl carbylamine	67.09	10.5	-250.4	605.1	597.2	599.3	10.5	55-77
	C_4H_7N	Propyl carbylamine	69.10	11.5	-266.3	639.6	637.8	633.9	11.5	55-77
	C_5H_9N	i-Butyl carbylamine	83.13	14.5	-279.1	796.0	793.3	792.7	14.5	55-77
	$C_6H_{11}N$	i-Amyl carbylamine	97.16	17.5	-288.2	959.5	951.6	94?.9	17.5	55-77
	~~C_8H_7N~~	~~Benzyl carbylamine~~	~~117.14~~	~~19.5~~	~~-266.3~~	~~1066.5~~	~~1050.3~~	1049.5	19.5	55-77
		$y' = 26.63 + 52.65x'$						$\Sigma x' = 101.5$ $\Sigma y' = 5983.6$ $\Sigma x'y' = 73,476.4$ $\Sigma x'^2 = 1,314.25$ $n = 9$		

TABLE 106

PRIMARY AMINES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	C_c^p, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	CH_5N	Methylamine	31.06	4.5	-231.8	255.1	254.1	250.4	4.5	55-99
	C_2H_7N	Ethylamine	45.08	7.5	-266.2	408.5	407.9	402.5	7.5	55-99
	C_3H_7N	Allylamine	57.09	9.5	-266.2	524.8	524.5	507.0	9.5	55-99
	C_3H_9N	Propylamine	59.11	10.5	-284.2	558.3	561.7	552.6	10.5	55-99
	$C_4H_{11}N$	n-Butylamine	73.14	13.5	-295.3	710.6	715.5	704.9	13.5	55-99
	"	i-Butylamine	"	"	"	713.6	712.9	710.5	13.5	55-99
	"	sec-Butylamine	"	"	"	713.0	"	709.8	13.5	55-99
	"	t-Butylamine	"	"	"	716.0	"	712.8	13.5	55-99
	C_6H_7N	Aniline	93.12	15.5	-266.3	810.6	809.1	813.9	15.5	5
	$C_5H_{13}N$	1-Amylamine	87.16	16.5	-302.9	866.8	867.1	863.3	16.5	55-99
	C_7H_9N	Benzylamine	107.15	18.5	-276.2	967.6	963.1	970.7	18.5	55-101, 55-147 (Av.)
	"	o-Toluidine	"	"	"	964.1	"	967.4	18.5	55-147
	"	m-Toluidine	"	"	"	965.3	"	968.4	18.5	55-147
	$C_6H_{15}N$	Hexylamine	101.19	19.5	-308.3	1022.2	1023.1	1016.5	19.5	55-99
	$C_7H_{15}N$	1-Methylcyclohexylamine-)	113.20	21.5	-303.9	1116.7	1118.9	1120.4	21.5	55-215
	$C_8H_{11}N$	2,4-Dimethylaniline	121.18	"	-283.9	1108.0	1115.3	1112.7	21.5	55-99
	$C_7H_{17}N$	Heptylamine	115.21	22.5	-312.5	1176.9	1176.9	1171.2	22.5	55-99
	$C_2H_{10}N_2O$	Ethylenediamine hydrate	78.12	8.0	-163.9	452.6	455.0	321.2	4.0	16
		$y' = 17.67 + 51.27x'$						$\Sigma x' =$	262.5	
								$\Sigma y' =$	13,776.5	
								$\Sigma x'y' =$	228,805.95	
								$\Sigma x'^2 =$	4372.25	
								$n =$	18	

TABLE 107

PRIMARY AMINES (gas)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	C_c^p, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	CH_5N	Methylamine	31.06	4.5	-231.8	258.1	257.5	252.6	4.5	55-223, 55-142 (Av.)
	C_2H_7N	Ethylamine	45.08	7.5	-266.2	413.1	413.4	407.6	7.5	55-223
	C_3H_7N	Allylamine	57.09	9.5	"	528.1	531.5	509.5	9.5	55-223
	C_3H_9N	Propylamine	59.11	10.5	-284.2	572.3	569.4	566.8	10.5	55-223
		$y' = 17.96 + 51.99x'$						$\Sigma x' =$	32.0	
								$\Sigma y' =$	1735.5	
								$\Sigma x'y' =$	14,975.85	
								$\Sigma x'^2 =$	277.0	
								$n =$	4	

TABLE 108

PRIMARY AMINES (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	C_c^p, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
	C_6H_7NO	p-Aminophenol	109.12	14.5	-212.6	760.0	757.7	760.6	14.5	55-97
	C_7H_9NO	p-Anisidine	123.15	17.5	-227.4	924.0	927.0	911.3	17.5	55-99
	C_7H_9N	p-Toluidine	107.15	18.5	-276.2	958.4	963.2	961.5	18.5	55-147
	$C_9H_{13}N$	Pseudocumidine	135.20	24.5	-289.9	1265.9	1274.1	1270.1	24.3	55-99
	$C_{10}H_9N$	1-Naphthylamine	143.18	"	-273.8	1263.5	1263.4	1278.4	24.5	55-99
	"	2-Naphthylamine	"	"	"	1261.0	"	1275.9	24.5	55-99
	$C_{12}H_{11}N$	2-Aminobiphenyl	169.22	29.5	-278.9	1532.4	1523.6	1547.1	29.5	18
	"	4-Aminobiphenyl	"	"	"	1524.1	"	1538.8	29.5	18
	$C_6H_8N_2$	p-Phenylenediamine	108.14	16.0	-235.7	839.8	837.3	421.6	8.0	57
	$C_{12}H_{12}N_2$	Benzidine	184.23	30.0	-260.5	1555.0	1558.1	787.0	15.0	99
	"	"	"	"	"	1556.0	"	785.3	15.0	55-100
	"	"	"	"	"	1560.9	"	787.7	15.0	55-147
		$y' = 4.26 + 52.00x'$						$\Sigma x'$	236.0	
								$\Sigma y' =$	12,323.3	
								$\Sigma x'y' =$	253,238.85	
								$\Sigma x'^2 =$	5139.0	
								$n =$	12	

TABLE 109

SECONDARY AMINES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_2H_7N	Dimethylamine	45.08	7.5	-266.2	416.7	413.7	411.0	7.5	55-99
	$C_4H_{11}N$	Diethylamine	73.14	13.5	-295.3	727.8	725.5	717.1	13.5	55-99
	C_7H_9N	Methylaniline	107.15	18.5	-276.4	970.9	976.5	980.0	18.5	55-[illegible]
	"	"	"	"	"	973.5	"	976.6	18.5	55-147
	$C_9H_{13}N$	Benzylethylamine	135.20	24.5	-289.9	1289.6	1288.6	1292.3	24.5	55-99
	$C_8H_{19}N$	Di-i-butylamine	129.24	25.5	-315.7	1344.4	1347.5	[illegible]	25.5	55-99
	$C_{10}H_{23}N$	Di-i-amylamine	157.29	31.5	-320.4	1660.4	1659.8	1655.6	31.5	55-99
		$y' = 13.34 + 51.96x'$						$\Sigma x' = 139.5$ $\Sigma y' = 7376.8$ $\Sigma x'y' = 167,050.3$ $\Sigma x'^2 = 3165.75$ $n = 7$		
	$C_8H_{11}N$	Ethylaniline	121.18	21.5	-283.9	1121.5	1132.6	-	-	55-99

TABLE 110

SECONDARY AMINES (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_{12}H_{11}N$	Diphenylamine	169.22	29.5	-278.9	1536.2	1532.0	1545.2	29.5	55-182
	"	"	"	"	"	1530.2	"	1542.7	29.5	55-99
	$C_{14}H_{15}N$	Dibenzylamine	197.27	35.5	-287.9	1853.0	1856.5	1865.1	35.5	55-99
	$C_{16}H_{13}N$	N-Phenyl-α-naphthylamine	219.27	38.5	-280.9	2003.8	1999.5	2034.3	38.5	55-99
	"	N-Phenyl-β-naphthylamine	"	"	"	1998.0	"	2023.5	38.5	55-99
		$y' = -44.9 + 53.90x'$						$\Sigma x' = 171.5$ $\Sigma y' = 9019.3$ $\Sigma x'y' = 313,925.15$ $\Sigma x'^2 = 5965.25$ $n = 5$		

TABLE 111

TERTIARY AMINES (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_3H_9N	Trimethylamine	59.11	10.5	-284.2	578.6	573.9	572.9	10.5	55-99
	$C_6H_{15}N$	Triethylamine	101.19	19.5	-308.3	1036.8	1040.3	1031.1	19.5	55-99
	$C_8H_{11}N$	Dimethylaniline	121.18	21.5	-283.9	1142.7	1139.0	1142.7	21.5	55-182
	$C_{10}H_{15}N$	Diethylaniline	149.23	27.5	-294.8	1457.6	1452.4	1454.1	27.5	55-182
	$C_{12}H_{27}N$	Tri-n-butylamine	185.34	37.5	-323.7	1973.6	1961.9	1964.2	37.5	55-99
	$C_{15}H_{33}N$	Tri-i-amylamine	227.42	46.5	-327.1	2469.3	2462.1	2451.1	46.5	55-99
		$y' = 20.40 + 52.16x'$						$\Sigma x' = 163.0$ $\Sigma y' = 8675.0$ $\Sigma x'y' = 278,616.7$ $\Sigma x'^2 = 5277.5$ $n = 6$		
	$C_{18}H_{15}N$	Triphenylamine (s)	245.31	43.5	-283.7	2267.8	2257.8(114)	-	-	55-182
	$C_{21}H_{21}N$	Tribenzylamine (s)	287.39	52.5	-292.3	2762.1	2737.9(114)	-	-	55-99

TABLE 112

AMIDES (liquid)

ADI NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_2H_4N_2O_2$	Formylurea	88.07	4.0	- 72.7	207.0	217.6	93.6	2.0	55-130
	$C_4H_8N_2O_4$	D-Tartramide	148.12	5.0	- 86.4	427.0	419.6	207.9	4.0	55-54
	"	meso-Tartramide	"	"	"	426.6	"	207.7	4.0	55-54
	$C_8H_{16}N_2O_4$	D-Tartaricdiethylamide	204.22	20.0	-156.7	1064.1	1065.7	513.5	10.0	55-54
	"	DL-Tartaricdiethylamide	"	"	"	1066.1	"	519.6	10.0	55-54
	"	meso-Tartaricdiethylamide	"	"	"	1065.3	"	520.1	10.0	55-54
		$y' = -6.47 + 52.68x'$						$\Sigma x' =$ 40.0 $\Sigma y' =$ 2068.4 $\Sigma x'y' =$ 17,441.6 $\Sigma x'^2 =$ 336.0 $n =$ 6		
	CH_3NO	Formamide	45.04	2.5	- 53.3	134.9	131.6	-	-	55-209

TABLE 113

AMIDES (solid)

ADI NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_2H_3NO_3$	Oxamic acid	89.05	2.5	- 44.9	[illegible]	146.8	137.4	2.5	55-130
	C_2H_5NO	Acetamide	59.07	5.5	-149.0	282.6	287.0	276.9	5.5	55-209
	$C_3H_5NO_3$	Methyl oxamate	103.08	"	- 85.4	305.4	300.8	295.9	5.5	55-184
	$C_3H_7NO_2$	Ethyl carbamate	89.09	7.5	-134.7	397.2	404.4	379.6	7.5	55-184
	C_3H_7NO	Propionamide	73.09	8.5	-186.1	439.9	443.7	434.2	8.5	55-209
	$C_4H_7NO_3$	Ethyl oxamate	117.10	"	-116.1	457.3	466.2	439.1	8.5	55-184
	C_4H_9NO	n-Butyramide	87.12	11.5	-211.8	596.0	600.5	590.3	11.5	55-209
	"	i-Butyramide	"	"	"	595.9	597.6	592.9	11.5	55-209
	$C_5H_{11}NO$	i-Valeramide	101.15	14.5	-229.4	751.5	[illegible]	748.2	14.5	55-209
	C_7H_7NO	Formanilide	121.13	16.5	-217.9	861.0	865.7	851.3	15.5	55-209
	"	Benzamide	"	"	"	848.0	852.8	852.0	16.5	5
	C_8H_9NO	Acetanilide	135.16	19.5	-230.8	1010.4	1012.4	1010.7	19.5	55-209
	$C_9H_9NO_3$	N-Benzoylglycine	179.17	"	-174.1	1012.4	1008.9	1016.2	19.5	55-208
	C_9H_7NO	N-Phenylpropiolamide	145.15	20.5	-266.0	1095.6	1099.2	1051.3	20.5	55-138
	$C_8H_{13}NO$	N-Amylpropiolamide	139.19	21.5	-247.2	1150.4	1140.2	1107.4	21.5	55-138
	$C_{10}H_{11}NO_4$	N-(p-Anisoyl)glycine	209.20	"	-214.4	1135.2	1128.1	1124.3	21.5	55-208
	$C_{10}H_{11}NO_3$	N-Benzoylalanine	193.20	22.5	-186.3	1168.1	1163.7	1173.8	22.5	55-208
	$C_9H_{11}NO$	Propionanilide	149.19	"	-241.3	1167.6	1169.1	1167.9	22.5	55-209
	$C_{10}H_{11}NO_3$	N-(o-Toluyl)glycine	193.20	"	-186.3	1167.7	1163.7	1173.4	22.5	55-208
	"	N-(m-Toluyl)glycine	"	"	"	1157.0	"	1172.7	22.5	55-208
	"	N-(p-Toluyl)glycine	"	"	"	1167.5	"	1173.2	22.5	55-208
	"	N-(Phenylacetyl)glycine	"	"	"	1164.9	"	1170.6	22.5	55-208
	$C_9H_{15}NO$	N-Hexylpropiolamide	153.22	24.5	-255.8	1308.0	1316.9	1265.0	24.5	55-138
	$C_{10}H_{13}NO_2$	Phenacetin	179.21	"	-218.7	1285.2	1259.5	1269.6	24.5	55-160
	$C_{11}H_{13}NO_3$	N-(o-Toluyl)alanine	207.22	25.5	-196.9	1321.7	1318.7	1329.1	25.5	55-208
	"	N-(p-Toluyl)alanine	"	"	"	1319.5	"	1326.[illegible]	25.5	55-208
	$C_{13}H_{11}NO$	Benzanilide	197.23	30.5	-247.4	1575.5	1566.9	1575.9	30.5	55-209
	$C_{16}H_{15}NO_3$	N-(Benzoyl)-N-phenylalanine	269.29	36.5	-216.9	1890.1	1876.9	1914.3	[illegible]	55-66
	CH_4N_2O	Urea	60.06	3.0	- 79.9	151.0	150.4	[illegible]	1.5	48
	"	"	"	"	"	151.3	"	[illegible]	1.5	134
	$C_2H_4N_2O_2$	Oxamide	88.07	4.0	- 72.7	[illegible]	[illegible]	[illegible]	2.0	55-184
	$C_3H_6N_2O_2$	Malonamide	102.09	7.0	-109.7	350.8	359.2	176.6	3.5	55-184
	$C_3H_8N_2O$	Ethylurea	88.11	9.0	-163.[illegible]	477.0	475.2	[illegible]	4.5	55-130
	$C_4H_8N_2O_2$	Succinamide	116.12	10.0	-137.6	509.2	516.0	[illegible]	5.0	55-184
	$C_5H_{10}N_2O_2$	N,N'-Dimethylmalonamide	130.15	13.0	-159.8	685.6	672.6	340.1	6.5	55-184
	$C_7H_{14}N_2O_2$	N,N'-Diethylmalonamide	158.20	19.0	-192.2	994.8	986.2	494.6	9.5	55-184
	$C_{13}H_{12}N_2O$	1,3-Diphenylurea	212.24	31.0	-233.7	1612.1	1600.9	809.[illegible]	15.5	55-184
	"	1,1-Diphenylurea	"	"	"	1614.5	1617.9	802.0	15.5	55-194
	$C_{16}H_{16}N_2O_2$	Succinanilide (sym)	268.30	38.0	-226.6	1970.4	1964.8	984.4	19.0	55-184
	$C_3H_4N_2O_4$	Oxaluric acid	132.08	4.0	- 18.5	207.5	[illegible]	68.7	1.33	55-130
	$C_3H_6N_2O_2$	Acetylurea	102.09	7.0	-109.7	360.[illegible]	352.8	118.[illegible]	2.33	55-130
		$y' = -6.03 + 52.$[illegible]x'						$\Sigma x' =$ 600.66 $\Sigma y' =$ 31,131.4 $\Sigma x'y' =$ 635,683.373 $\Sigma x'^2 =$ 12,240.1978 $n =$ 41		
	$C_3H_8N_2O_3$	Dimethylolurea	120.11	7.0	- 93.2	391.0	406.1	-	-	121
	$C_{15}H_{16}N_2O$	1,3-Dimethyl-1,3-diphenyl-urea	240.29	37.0	-216.4	1953.0	1945.3	-	-	141
	$C_{17}H_{20}N_2O$	1,3-Diethyl-1,3-diphenyl-urea	268.35	43.0	-256.4	2266.7	2218.5	-	-	141

TABLE 114

HYDRAZINES (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c, KCAL/MOLE OBSERVED	Q_c, KCAL/MOLE CALCULATED	Y'	X'	REF.
352	$H_5N_3O_3$	Hydrazine mononitrate	95.06	+ 0.5	+ 8.4	112.2	120.9	127.0	2.0	96
956	$CH_6N_6O_2$	1-Amino-3-nitroguanidine	119.09	+ 2.5	- 33.6	270.1	265.1	267.5	2.5	77
	$C_2H_6N_2O_4$	Hydrazine hydrogen oxalate	122.08	3.0	- 39.3	149.1	178.4	147.2	2.0	96
355	$C_2H_4N_{10}$	5,5'-Hydrazo-1H-tetrazole	168.13	6.0	- 57.1	469.7	479.0	335.3	6.0	92
334	$C_6H_6N_4O_4$	2,4-Dinitrophenylhydrazine	198.14	11.0	- 80.8	797.4	789.5	612.2	11.0	58
511	$C_6H_8N_2$	Phenylhydrazine	108.14	16.0	-236.7	871.7	866.5	869.1	16.0	5
"	"	"	"	"	"	875.4	"	873.5	16.0	55-100
590	$C_7H_{10}N_2$	as-Methylphenylhydrazine	122.10	19.0	-249.0	1038.3	1033.0	1025.3	19.0	55-100
693	$C_8H_{12}N_4$	2,2'-Hydrazobis-2-butyronitrile	166.22	23.0	-221.4	1259.2	1257.5	1219.7	23.0	77
	$C_{12}H_{10}N_4O_4$	4,4'-Dinitrohydrazobenzene	274.23	25.0	-145.9	1496.4	1509.0	1319.4	25.0	26
591	$C_{12}H_{12}N_2$	Hydrazobenzene	184.23	30.0	-260.5	1590.4	1591.2	1591.1	30.0	99
"	"	"	"	"	"	1597.5	"	1588.5	30.0	132
"	"	"	"	"	"	1591.4	"	1597.1	30.0	25
"	"	"	"	"	"	1597.3	"	1594.0	30.0	55-100
"	"	"	"	"	"	1598.5	"	1595.5	30.0	55-147
	$C_{12}H_{14}N_2I_2$	Hydrazobenzene dihydroiodide	440.09	31.0	-112.7	1644.8	1613.2	1593.5	30.0	99
592	$C_{24}H_{20}N_2$	Tetraphenylhydrazine	336.42	58.0	-275.0	3060.7	3066.2	[illegible]	58.0	5
531	$CH_8N_6O_3$	1,3-Diaminoguanidine mononitrate	152.12	3.0	- 31.6	329.8	333.4	173.6	2.75	77
	$CH_8N_7O_3$	1,2,3-Triaminoguanidine mononitrate	167.14	3.5	- 33.5	398.6	411.0	191.3	2.0	91
		$y' = 32.16 + 57.98x'$								
								$\Sigma x' = 365.25$		
								$\Sigma y' = 19,666.4$		
								$\Sigma x'y' = 582,386.25$		
								$\Sigma x'^2 = 10,973.8125$		
								$n = 19$		
353	H_4N_2	Hydrazine (liq)	32.05	2.0	- 99.8	148.6	142.2(s)	-	-	50
691	H_6N_2O	Hydrazine hydrate (liq)	50.06	2.0	- 63.9	116.9	116.2(s)	-	-	50
1392	CH_6N_2	Methylhydrazine (liq)	46.07	5.0	-173.6	311.9	311.4(s)	-	-	26
354	$C_2H_4N_{10}$	5,5'-Hydrazo-1H-tetrazole	168.13	6.0	- 57.1	459.9	479.0	-	-	77
511	$C_6H_8N_2$	Phenylhydrazine	108.14	16.0	-236.7	805.4	866.5	-	-	55-147
696	$C_{14}H_{12}N_2O_2$	N,N'-Dibenzamide	240.25	32.0	-213.1	1675.5	1666.5	-	-	5
695	$C_{16}H_{16}N_2O_2$	N,N'-Diacetanilide	268.30	38.0	-466.6	2006.3	1995.7	-	-	99

TABLE 115

HYDRAZIDES (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c, KCAL/MOLE OBSERVED	Q_c, KCAL/MOLE CALCULATED	Y'	X'	REF.
694	$C_{14}H_{14}N_2O$	Acetic 1,2-diphenylhydrazide	226.27	34.0	-240.4	1792.9	1792.4	1796.3	34.0	99
537	$C_3H_8N_4O_5$	Carbohydrazide hydrogen oxalate	180.13	5.0	- 44.4	314.6	304.0	165.3	2.5	96
552	$C_2H_6N_4O_2$	Oxalic dihydrazide	118.10	5.0	- 67.7	327.9	325.7	150.6	2.5	57
"	"	"	"	"	"	325.7	"	150.0	2.5	92
	$C_2H_7N_5O_2$	Diaminobiuret	133.12	5.5	- 66.1	343.5	310.5	174.5	2.75	96
697	$C_3H_8N_4O_2$	Malonic dihydrazide	132.13	8.0	- 96.9	476.3	481.5	235.3	4.0	57
698	$C_4H_{10}N_4O_2$	Succinic dihydrazide	146.15	11.0	-120.4	639.6	537.2	312.5	5.5	57
		$y' = 30.18 + 51.93x'$								
								$\Sigma x' = 53.75$		
								$\Sigma y' = 3602.5$		
								$\Sigma x'y' = 65,423.775$		
								$\Sigma x'^2 =$ [illegible]		
								$n = 7$		

TABLE 116

AZO (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	G_c°, KCAL/MOLE OBSERVED	G_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_6H_{14}N_2$	Azo-i-propane (liq)	114.19	19.0	-266.2	1053.4	1050.7	1059.7	19.0	25
	$C_8H_{12}N_4$	2,2'-Azobis-i-butyronitrile	164.21	22.0	-233.8	1217.0	1230.3	1180.0	22.0	77
	$C_{12}H_{10}N_2O$	p-Hydroxyazobenzene	198.22	28.0	-266.0	1502.0	1456.3	1515.7	28.0	55-101
	$C_{12}H_{10}N_2$	Azobenzene	182.22	29.0	-254.6	1544.6	1518.9	1557.2	29.0	139
	"	"	"	"	"	1555.2	"	1567.8	29.0	55-147
	"	"	"	"	"	1552.6	"	1565.3	29.0	55-101
	"	"	"	"	"	1545.9	"	1558.5	29.0	55-217
	$C_{12}H_{11}N_3$	p-Aminoazobenzene	197.23	29.5	-239.3	1574.0	1576.6	1584.6	29.5	55-101
	$C_{12}H_{12}N_4$	2,4-Diaminoazobenzene	212.25	30.0	-266.1	1597.4	1600.6	1603.7	30.0	55-101
	$C_{14}H_{14}N_2O_2$	p-Azoanisole	242.27	33.0	-217.9	1796.4	1794.6	1777.1	33.0	55-101
	$C_{16}H_{18}N_2O_2$	p-Azophenetole	270.32	39.0	-230.8	2100.0	2095.6	2080.2	39.0	55-101
	$C_{25}H_{20}N_2$	Phenylazo(triphenylmethane)	348.43	60.0	-275.5	3171.	3127.4	3203.0	60.0	152
	$C_{26}H_{22}N_2$	Benzylazo(triphenylmethane)	362.45	63.0	-278.1	3238.	3251.8	3267.0	63.0	152

$y' = 69.42 + 51.45x'$

$\Sigma x' = 439.5$
$\Sigma y' = 23,544.7$
$\Sigma x'y' = 802,282.0$
$\Sigma x'^2 = 16,942.25$
$n = 13$

TABLE 117

AZOXYS (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	G_c°, KCAL/MOLE OBSERVED	G_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_{12}H_{10}N_2O$	Azoxybenzene	198.22	28.0	-266.0	1534.5	1511.7	1547.1	28.0	55-101
	"	"	"	"	"	1530.1	"	1542.7	28.0	55-147
	$C_{14}H_{16}N_4O$	m-Azoxytoluidine	256.30	35.0	-218.5	1903.4	1907.4	1909.8	35.0	55-101
	$C_{16}H_{18}N_2O_3$	p-Azoxyphenetole	286.32	38.0	-212.3	2078.4	2071.8	2078.7	38.0	55-101
	"	o-Azoxyphenetole	"	"	"	2068.0	"	2068.3	38.0	55-101

$y' = 66.47 + 52.78x'$

$\Sigma x' = 167.[illegible]$
$\Sigma y' = 914[illegible].60$
$\Sigma x'y' = 310,[illegible]43.40$
$\Sigma x'^2 = 5681.0$
$n = 5$

TABLE 118

GUANIDINES (solids)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^v, KCAL/MOLE OBSERVED	Q_c^v, KCAL/MOLE CALCULATED	Y'	X'	REF.
628	[illegible]	1-Nitro-3-(2,2,2-trinitro-ethyl)guanidine	267.1[illegible]	0.5	- 3.0	432.5	432.6	26.4	0.5	128-1
152	$CH_4N_4O_2$	Nitroguanidine	104.07	2.0	- 30.7	208.5	206.5	106.5	2.0	77
"	"	"	"	"	"	208.8	"	106.2	2.0	23
"	"	"	"			210.2	"	107.6	2.0	84
"	"	"	"			207.8	"	105.2	2.0	124-3
"	"	"	"			210.3	"	107.7	2.0	74
"	"	"	"	"		210.0	"	107.4	2.0	94
114	$CH_6N_4O_3$	Guanidine nitrate	122.09	"	[illegible]2	208.2	211.7	229.5	4.5	174
116	$C_2H_5N_5O_3$	1-Guanyl-3-nitrourea	99.10	3.5	[illegible]5.5	288.9	285.6	184.7	3.5	94, 128-4
[illegible]	[illegible]	~~Guanylurea nitrate~~	165.12	"	- 33.9	295.1	263.7	321.0	6.0	94, 128-4
630	[illegible]	1-Nitro-3-(2,3-dihydroxy-propyl)guanidine dinitrate	268.15	4.0	- 23.9	584.0	585.4	205.8	4.0	128-1
625	[illegible]	1-Nitro-3-(1-hydroxyethyl)-guanidine nitrate	193.13	4.5	- 37.3	473.4	482.0	294.6	4.5	128-1
471	$C_2H_6N_4O_2$	1-Methyl-3-nitroguanidine	113.10	5.0	- 77.7	376.6	377.1	258.3	5.0	84
550	$C_2H_4N_4$	Cyanoguanidine (dicyandiamide)	84.08	6.0	-114.2	330.7	337.9	304.4	6.0	121
"	"	"	"	"	"	327.2	"	300.[illegible]	6.0	92
667	$C_3H_8N_4O_2$	1-Ethyl-3-nitroguanidine	132.13	8.0	- 96.9	530.3	532.3	411.7	8.0	84
	$C_4H_9N_3O_2$	Creatine	131.14	10.5	-123.1	555.1	561.5	536.3	10.5	49
	$C_4H_7N_3O$	Creatinine	113.12	"	-148.5	558.1	561.1	530.7	10.5	49
668	$C_4H_{10}N_4O_2$	1-(n-Propyl)-3-nitroguanidine	146.15	11.0	-120.4	683.7	687.3	569.9	11.0	84
669	$C_5H_{12}N_4O_2$	1-(n-Butyl)-3-nitroguanidine	160.18	14.0	-139.8	844.8	842.4	725.3	14.0	84
670	$C_6H_{14}N_4O_2$	1-(n-Amyl)-3-nitroguanidine	174.20	17.0	-156.1	1004	997.4	884.8	17.0	84
622	$C_5H_{13}N_9O_7$	1,1'-(2-Hydroxytrimethylene)-bis(3-nitroguanidine) mononitrate	309.21	9.5	- 44.0	601.1	602.9	219.2	4.25	128-1

$y' = 0.68 + 51.62x'$

$\Sigma x' = 127.25$
$\Sigma y' = 6583.5$
$\Sigma x'y' = 58,653.4$
$\Sigma x'^2 = 1134.5625$
$n = 22$

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	OBSERVED	CALCULATED	Y'	X'	REF.
152	$CH_4N_4O_2$	Nitroguanidine	104.07	2.0	- 30.7	209.8	206.5	-	-	56
631	[illegible]	1-Nitro-3-(2-hydroxyethyl)-guanidine nitrate	193.13	4.5	- 37.3	462.7	482.0	-	-	95-3
543	[illegible]	N-Guanylcarbamic acid	231.09	5.5	- 67.1	339.7	286.3	-	-	56
	$C_3H_{12}N_6O_3$	Di(guanidine) carbonate	180.17	9.0	- 79.9	459.8	-	-	-	33

TABLE 122

ALIPHATIC NITROS (solid)

AOL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	U_c°, KCAL/MOLE OBSERVED	U_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
676	$(C_3H_5NO_2)_n$	2-Nitropropene polymer	87.08	6.5	-119.4	422.2	429.5	319.6	6.5	128-3
192	$C_7H_5N_3O_6$	α, α, m-Trinitrotoluene	227.13	10.5	- 74.0	818.1	809.7	356.9	5.25	65
	$C_9H_{11}NO_2$	α-Nitromesitylene	165.19	21.5	-208.2	1194.3	1193.2	1197.0	21.5	55-243
574	$C_3H_6N_2O_6$	2,2-Dinitro-1,3-propanediol	166.09	3.0	- 28.9	365.6	363.6	170.9	1.5	128-2
77	$C_3H_6N_2O_5$	2,2-Dinitro-1-propanol	150.09	4.0	- 42.6	422.8	425.9	200.1	2.0	1
57	$C_4H_2N_2O_5$	2,5-Dinitrofuran	158.07	4.0	- 40.5	421.2	427.7	193.4	2.0	65
367	$C_3H_6N_2O_4$	2,2-Dinitropropane	134.09	5.0	- 59.7	441.4	446.3	217.9	2.5	63
651	$C_4H_8N_2O_6$	3,3-Dinitro-2,1-butanediol	180.12	6.0	- 53.3	500.6	514.9	241.7	3.0	128-2
600	$C_6H_4N_2O_5$	2-Nitro-5-(2-nitrovinyl)-furan	184.11	9.0	- 78.2	678.3	693.0	316.8	4.5	65
59	$C_5H_{10}N_2O_4$	2,2-Dimethyl-1,1-dinitropropane	162.15	11.0	-108.5	752.0	754.0	374.5	5.5	65
"	"	"	"	"	"	747.2	"	372.1	5.5	79
575	$C_7H_{10}N_2O_8$	4,4-Dinitropimelic acid	250.17	"	- 70.4	764.0	749.0	351.0	5.5	128-2
655	$C_5H_{12}N_4O_4$	3,3-Dinitro-1,5-pentanediamine	192.18	12.0	- 99.9	848.8	815.7	417.8	6.0	128-2
"	"		"	"	"	833.1	"	412.9	6.0	128-2
602	$C_7H_6N_2O_4$	α, α-Dinitrotoluene	182.13	13.0	-114.2	862.2	850.3	432.4	6.5	65
52	$C_6H_{12}N_2O_4$	2,3-Dimethyl-2,3-dinitrobutane	176.17	14.0	-127.2	887.7	908.5	442.2	7.0	128-3
"	"		"	"	"	872.0	"	444.4	7.0	79
"	"		"			[illegible]		447.0	7.0	79
265	$C_5H_9N_3O_6$	2-Methyl-2,3,3-trinitrobutane	207.15	8.5	- 65.7	699.1	718.0	506.3	2.833	79
570	$C_6H_{11}N_3O_6$	2-Methyl-2,3,3-trinitropentane	221.17	11.5	- 83.2	871.4	872.4	249.5	3.833	79
343	$C_4H_6N_4O_8$	2,2,3,3-Tetranitrobutane	238.12	3.0	- 20.2	521.0	531.3	133.3	0.75	71
657	$C_5H_8N_4O_{10}$	2,2,4,4-Tetranitro-1,5-pentanediol	284.15	4.0	- 22.5	606.0	600.5	146.1	1.00	128-2
653	$C_6H_8N_4O_{10}$	2,2,4,4-Tetranitro-1-butanol acetate	296.16	5.0	- 32.4	598.3	597.7	153.0	1.25	128-2
755	$C_7H_{10}N_4O_{10}$	Methyl-4,4,6,6-tetranitrocaproate	310.18	9.0	- 46.4	865.5	850.[illegible]	217.4	2.75	128-2
		$y' = 92.63 + 51.40x'$								
								$\Sigma x' = 116.915$		
								$\Sigma y' = 8237.5$		
								$\Sigma x'y' = 60,269.1678$		
								$\Sigma x'^2 = 961.45278$		
								$n = 24$		
179	$(C_2H_3NO_2)_n$	Nitroethylene polymer	73.05	3.5	- 76.7	266.1	278.4	-	-	128-3
848	$C_4H_9NO_5$	Tris(hydroxymethyl)nitromethane	151.12	7.5	- 79.4	509.3	505.2	-	-	31a
1676	$C_4H_9NO_4$	2-Nitro-2-methyl-1,3-propanediol	135.12	8.5	-100.7	545.0	552.5	-	-	31a
	$C_4H_9NO_3$	2-Nitro-2-methyl-1-propanol	119.12	9.5	-127.6	545.6	552.8	-	-	31a
1771	$C_5H_{11}NO_4$	2-Ethyl-2-nitro-1,3-propanediol	149.15	11.5	-123.4	700.6	704.7	-	-	31a
	$C_6H_{13}NO_4$	2-Nitro-2-propyl-1,3-propanediol	163.17	14.5	-142.2	853.9	859.1	-	-	31a
	"	2-Nitro-2-i-propyl-1,3-propanediol	"	"	"	859.4	"	-	-	31a
	$C_{10}H_{13}NO_3$	2-Nitro-2-methyl-1-phenyl-1-propanol	195.21	23.5	-192.6	1358.7	1364.5	-	-	31a
	"	2-Nitro-2-methyl-1-phenyl-1-propanol	"	"	"	1301.5	"	-	-	31a
397	$C_3H_4N_2O_4$	2,2-Dinitropropene	134.09	5.0	- 59.7	427.8	446.3	-		65

TABLE 123

AROMATIC NITRO (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c, KCAL/MOLE OBSERVED	Q_c, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_6H_3F_2NO_2$	2,[illegible]-Difluoronitrobenzene	159.09	10.5	-105.6	671.5	665.1	647.0	10.5	138
	$C_6H_4FNO_2$	p-Fluoronitrobenzene	141.10	11.5	-130.4	717.2	716.6	692.9	11.5	138
	"	m-Fluoronitrobenzene	"	"	"	706.0	"	691.7	11.5	138
515	$C_6H_5NO_2$	Nitrobenzene	123.11	12.5	-162.5	734.7	740.5	711.[illegible]	12.5	137
"	"	"	"	"	"	740.3	"	713.6	12.5	39
961	$C_7H_4F_3NO_2$	ω,ω,ω-Trifluoro-m-nitrotoluene	191.11	"	-104.7	770.6	771.1	743.5	12.5	138
[illegible]	$C_7H_7NO_2$	m-Nitrotoluene	137.13	15.5	-180.9	893.9	895.3	897.2	15.5	39
"	"	m- "	"	"	"	[illegible]	"	892.9	15.5	137
	"	o-Nitrotoluene	"	"	"	897.9	"	901.2	15.5	39
560	$C_8H_9NO_3$	o-Nitrophenetole	167.16	17.5	-167.5	1021.2	1015.2	1000.5	17.5	137
		$y' = 97.85 + 51.69x'$						$\Sigma x' =$	135.0	
								$\Sigma y' =$	7956.9	
								$\Sigma x'y' =$	109,695.05	
								$\Sigma x'^2 =$	1870.5	
								$n =$	10	
	$C_9H_{10}N_2O_4$	m,[illegible]-Dinitromesitylene	210.19	19.0	-114.6	1155.7	1156.0	-	-	55-243

TABLE 124

AROMATIC NITRO (solid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c, KCAL/MOLE OBSERVED	Q_c, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_6H_4FNO_3$	4-Fluoro-2-nitrophenol	157.10	10.5	-106.9	652.5	651.5	635.8	10.5	138
509	$C_6H_5NO_3$	p-Nitrophenol	139.11	11.5	-132.3	687.1	686.6	687.0	11.5	39
"	"	p- "	"	"	"	685.2	"	684.1	11.5	137
"	"	p- "	"	"	"	686.8	"	684.7	11.5	55-131
558	"	m-Nitrophenol	"	"	"	684.4	"	[illegible]	11.5	137
557	"	o-Nitrophenol	"	"	"	687.9	"	687.8	11.5	55-131
"	"	o- "	"	"	"	[illegible]	"	[illegible]	11.5	39
"	"	o- "	"	"	"	688.4	"	604.3	11.5	137
	$C_6H_4FNO_2$	p-Fluoronitrobenzene	141.10	"	-130.4	717.7	699.9	609.7	11.5	138
	$C_6H_5FN_2O_2$	4-Fluoro-3-nitroaniline	156.12	12.0	-123.0	[illegible]	720.9	[illegible]	[illegible]	[illegible]
	$C_7H_5NO_4$	o-Nitrobenzoic acid	167.12	12.5	-119.7	729.8	730.1	737.3	12.5	55-131
	"	m-Nitrobenzoic acid	"	"	"	726.4	"	733.9	12.5	55-58
	"	m- "	"	"	"	727.1	"	736.6	12.5	55-151
	"	p-Nitrobenzoic acid	"	"	"	723.3	"	735.8	12.5	55-58
	"	p- "	"	"	"	728.3	"	735.8	12.5	55-151
552	$C_6H_6N_2O_2$	o-Nitroaniline	138.12	13.0	-150.6	765.9	763.0	756.1	13.0	137
597	"	m-Nitroaniline	"	"	"	766.3	"	766.5	13.0	137
563	"	p-Nitroaniline	"	"	"	760.2	"	760.1	13.0	137
572	$C_7H_5NO_3$	o-Nitrobenzaldehyde	151.12	13.5	-142.9	792.7	791.7	785.9	13.5	115
"	"	p- "	"	"	"	801.0	"	794.2	13.5	75
1979	"	m-Nitrobenzaldehyde	"	"	"	800.4	"	793.6	13.5	55-131
616	$C_7H_7NO_2$	p-Nitrotoluene	137.13	15.5	-180.9	887.5	887.9	872.8	15.5	39
	$C_7H_8N_2O_2$	5-Nitro-o-toluidine	152.15	16.0	-160.3	910.4	918.6	910.7	16.0	138
	"	3-Nitro-p-toluidine	"	"	"	915.1	"	915.4	16.0	138
	$C_7H_8N_2O_2$	N-Methyl-p-nitroaniline	152.15	"	-168.3	915.2	932.2	912.1	16.0	39
	$C_8H_7FN_2O_3$	4-Fluoro-3-nitroacetanilide	198.15	"	-129.2	9[illegible]	929.4	922.1	16.0	138
	$C_8H_8FNO_3$	4-Fluoro-2-nitrophenetole	185.15	16.5	-112.6	980.9	975.1	970.7	16.5	138
560	$C_8H_9NO_3$	o-Nitrophenetole	167.16	17.5	-167.5	1017.5	1009.3	1004.8	17.5	137
[illegible]	"	m-Nitrophenetole	"	"	"	1009.2	"	996.5	17.5	137
562	"	p-Nitrophenetole	"	"	"	1006.0	"	993.3	17.5	137
	$C_9H_7NO_4$	o-Nitrocinnamic acid	193.15	"	-1[illegible]	999.0	1003.5	992.1	17.5	55-226
	"	m-Nitrocinnamic acid	"	"	"	995.6	"	988.7	17.5	55-226
	"	p-Nitrocinnamic acid	"	"	"	996.5	"	989.6	17.5	55-226
	$C_9H_{11}NO_2$	Nitromesitylene	165.19	21.5	-208.2	1204.7	1193.4	1,197.4	21.5	55-243
	$C_{12}H_9NO_2$	m-Nitrobiphenyl	199.20	26.5	-212.9	1178.7	1165.9	1173.0	26.5	18
	"	p-Nitrobiphenyl	"	"	"	1140.1	"	1144.1	26.5	18
	$C_{14}H_{11}NO_2$	4-Nitrostilbene (cis)	225.24	31.5	-223.8	1723.2	1720.9	1722.4	31.5	4
	"	4-Nitrostilbene (trans)	"	"	"	1716.7	"	1715.4	31.5	4
	$C_6H_3FN_2O_4$	1-Fluoro-2,4-dinitrobenzene	186.10	9.0	-77.4	668.[illegible]	660.7	325.9	4.5	138
71	$C_6H_4N_2O_5$	2,4-Dinitrophenol	184.11	"	-78.2	647.6	650.2	[illegible]	4.5	138
"	"	2,4- "	"	"	"	644.2	"	324.3	4.5	39
"	"	2,4- "	"	"	"	645.5	"	322.5	4.5	10
"	"	2,4- "	"	"	"	[illegible]	"	323.1	4.5	23
346	"	2,6-Dinitrophenol	"	"	"	651.5	"	325.5	4.5	10

TABLE 124

AROMATIC NITRO (solid) (Cont'd)

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
45	$C_6H_4N_2O_4$	m-Dinitrobenzene	168.11	10.0	- 95.2	696.3	697.5	350.0	5.0	110
	"	m- "	"	"	"	697.1	"	350.5	5.0	15
	"	m- "	"	"	"	699.3	"	351.8	5.0	39
	"	m- "	"	"	"	693.4	"	348.6	5.0	9
	"	m- "	"	"	"	696.3	"	350.0	5.0	104
	"	m- "	"	"	"	694.8	"	349.3	5.0	143
	"	m- "	"	"	"	695.5	"	349.3	5.0	23
	"	m- "	"	"	"	695.1	"	349.4	5.0	137
	"	o-Dinitrobenzene	"	"	"	703.2	"	353.5	5.0	15
	"	o- "	"	"	"	701.9	"	353.4	5.0	37
	"	p-Dinitrobenzene	"	"	"	695.1	"	349.5	5.0	15
	"	p- "	"	"	"	692.9	"	348.3	5.0	37
46	$C_7H_6N_2O_5$	2,4-Dinitroanisole	198.13	12.0	- 96.9	817.7	816.8	403.8	6.0	23
"	"	2,4- "	"	"	"	819.1	"	404.5	6.0	10
84	$C_7H_6N_2O_4$	2,4-Dinitrotoluene	182.13	11.0	-114.2	847.1	852.8	425.4	6.5	23
	"	2,4- "	"	"	"	847.2	"	425.3	6.5	8
	$C_7H_7N_3O_4$	N-Methyl-2,4-dinitroaniline	197.15	13.5	-129.6	895.2	895.2	446.0	6.75	39
156	$C_8H_8N_2O_5$	2,4-Dinitrophenetole	212.16	15.0	-113.1	972.4	972.0	482.[illegible]	7.5	19
"	"	2,4- "	"	"	"	972.9	"	480.3	7.5	23
	$C_8H_8N_2O_4$	2,4-Dinitro-m-xylene	196.16	16.0	-130.5	1006.2	1004.7	504.9	8.0	8
86	"	4,6-Dinitro-m-xylene	"	"	"	1002.2	"	503.9	8.0	8
604	$C_{10}H_{13}N_3O_7$	2-(2,4-Dinitroanilino)-2-hydroxymethyl-1,3-propanediol	287.23	19.5	-108.6	1222.[illegible]	1231.6	591.9	9.75	65
603	$C_{10}H_{13}N_3O_6$	N-(2,4-Dinitrophenyl)-diethanolamine	271.23	20.5	-120.9	1274.7	1275.2	619.2	10.25	65
1136	$C_{10}H_{13}N_3O_6$	2-(2,4-Dinitroanilino)-2-methyl-1,3-propanediol	271.23	"	-120.9	1266.9	1273.9	614.4	10.25	65
216	$C_6H_3N_3O_7$	2,4,6-Trinitrophenol	229.11	6.5	- 45.4	616.0	613.3	294.6	2.167	23
"	"	2,4,6- "	"	"	"	614.2	"	294.3	2.167	35
"	"	2,4,6- "	"	"	"	611.0	"	293.7	2.167	110
"	"	2,4,6- "	"	"	"	615.1	"	294.6	2.167	10
"	"	2,4,6- "	"	"	"	611.9	"	293.6	2.167	36
274	$C_6H_3N_3O_6$	1,3,5-Trinitrobenzene	213.11	7.5	- 56.3	657.7	660.3	220.5	2.50	143
"	"	1,3,5- "	"	"	"	657.0	"	220.6	2.50	23
"	"	1,3,5- "	"	"	"	659.8	"	221.[illegible]	2.50	35
"	$C_7H_3N_3O_7$	2,4,6-Trinitrobenzaldehyde	241.12	8.5	- 56.4	727.1	722.7	240.7	2.833	110
277	$C_7H_5N_3O_7$	2,4,6-Trinitro-m-cresol	243.13	9.5	- 62.5	768.9	768.2	256.1	3.167	10
"	"	2,4,6- "	"	"	"	769.3	"	256.2	3.167	23
271	$C_7H_5N_3O_7$	2,4,6-Trinitroanisole	243.13	"	- 62.5	784.4	774.2	[illegible]	3.167	110
313	$C_7H_5N_3O_6$	2,4,6-Trinitrotoluene	227.13	10.5	- 74.0	814.0	815.6	[illegible]	3.50	143
"	"	2,4,6- "	"	"	"	815.3	"	[illegible]	3.50	110
"	"	2,4,6- "	"	"	"	814.4	"	[illegible]	3.50	23
"	"	2,4,6- "	"	"	"	814.3	"	[illegible]	3.50	86
"	"	2,4,6- "	"	"	"	814.3	"	[illegible]	3.50	8
292	$C_7H_6N_4O_6$	N-Methyl-2,4,6-trinitroaniline	242.15	11.0	- 72.7	858.3	858.[illegible]	[illegible]	3.667	37
294	$C_8H_7N_3O_7$	2,4,6-Trinitrophenetole	257.16	12.5	- 78.[illegible]	943.7	935.0	[illegible]	4.167	10
"	"	2,4,6- "	"	"	"	933.0	"	[illegible]	4.167	143
"	"	2,4,6- "	"	"	"	943.7	"	320.5	4.167	23
318	$C_8H_7N_3O_6$	2,4,6-Trinitro-m-xylene	241.16	13.5	- 89.6	957.7	968.5	324.5	4.50	8
"	"	2,4,6- "	"	"	"	971.6	"	325.5	4.50	110
"	"	2,4,6- "	"	"	"	971.7	"	325.9	4.50	143
"	"	2,4,6- "	"	"	"	964.3	"	324.7	4.50	23
325	$C_9H_7N_3O_7$	Allyl picrate	269.17	14.5	- 56.2	1066.7	1052.5	356.8	4.833	71
326	$C_9H_9N_3O_7$	n-Propyl picrate	271.17	15.5	- 91.4	1103.5	1090.1	361.7	5.167	71
233	$C_6H_3N_5O_8$	2,3,4,6 Tetranitroaniline	273.12	5.5	- 32.2	655.0	653.9	163.8	1.375	110
125	$C_{12}H_5N_7O_{12}$	2,2',4,4',6,6'-Hexanitrodiphenylamine	439.22	14.5	- 52.8	1323	1321.7	217.5	2.667	56
"	"	2,2',4,4',6,6'- "	"	"	"	1317.6	"	219.1	2.167	110
"	"	2,2',4,4',6,6'- "	"	"	"	1310.6	"	217.9	2.667	65
	$C_{10}H_7NO_2$	Nitronaphthalene	173.16	21.5	-193.7	1190.5	1190.2	1203.6	21.5	110
480	"	1-Nitronaphthalene	"	"	"	1190.1	"	1203.2	21.5	7
481	$C_{10}H_6N_2O_4$	1,5-Dinitronaphthalene	218.16	19.0	-139.3	1154.6	1156.8	583.1	9.5	110
"	"	1,5- "	"	"	"	1152.6	"	582.1	9.5	7
"	"	1,5- "	"	"	"	1157.3	"	584.5	9.5	143
482	"	1,8-Dinitronaphthalene	"	"	"	1154.6	"	583.3	9.5	110
"	"	1,8- "	"	"	"	1151.9	"	[illegible]	9.5	7
"	"	1,8- "	"	"	"	1164.1	"	587.8	9.5	143
483	$C_{10}H_5N_3O_6$	1,3,5-Trinitronaphthalene	263.16	16.5	-100.3	1117.9	1117.2	374.0	5.5	7
493	"	1,3,8-Trinitronaphthalene	"	"	"	1122.6	"	377.4	5.5	8
"	"	1,3,8- "	"	"	"	1119.3	"	373.[illegible]	5.5	110
484	"	1,4,5-Trinitronaphthalene	"	"	"	1120.3	"	377.0	5.5	7

TABLE 274

AROMATIC NITROS (solid) (Cont'd)

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c, KCAL/MOLE OBSERVED	Q_c, KCAL/MOLE CALCULATED	Y'	X'	REF.
[illegible]	[illegible]	1,3,6,8-Tetranitronaphthalene	308.16	14.0	- 72.7	1002.3	1003.7	272.9	3.5	85
		$y' = $ [illegible]$.71 + $[illegible]$x'$					$\Sigma x' = 1304.113$ $\Sigma y' = 62,310.2$ $\Sigma x'y' = 790,547.6372$ $\Sigma x'^2 = 13,505.580227$ $n = 113$			
[illegible]	$C_6H_5NO_3$	p-Nitrophenol	139.11	11.5	2.3	680.[illegible]	686.6	-	-	110
	$C_7H_5NO_4$	o-Nitrobenzoic acid	167.12	12.5		735.0	730.7	-	-	55-152
507	$C_6H_6N_2O_2$	m-Nitroaniline	138.12	13.0		754.1	763.3	-	-	110
	[illegible]	β,p-Dinitrostyrene	194.14	15.0	[illegible].6	957.4	950.7	-	-	55-226
		β,o-Dinitrostyrene	"	"	"	962.6	"	-	-	55-226
[illegible]	$C_8H_8N_2O_3$	o-Nitroacetanilide	180.16	17.0	-151.0	974.1	969.2	-	-	137
555	"	m-Nitroacetanilide	"	"	"	[illegible].6	"	-	-	137
566	"	p-Nitroacetanilide	"	"	"	950.2	"	-	-	137
	$C_{14}H_9NO_4$	p-Nitrobenzil	255.22	28.5	-178.[illegible]	1[illegible].9	1555.9	-	-	12
	$C_{16}H_{13}NO_4$	p-Nitroacetylbenzoin	297.26	33.5	-180.3	1664.3	1612.4	-	-	12
	[illegible]	p-Nitrobenzoylbenzoin	360.32	44.5	[illegible]	[illegible]		-	-	12
814	$C_{14}H_{10}N_2O_4$	4,4'-Dinitrostilbene, cis	270.24	29.0	-171.7	1675.3	1684.3	-	-	4
"		4,4'- " , trans	"	"	"	1670.7	"	-	-	4
	$C_{19}H_{13}N_3O_7$	Tris(nitrophenyl)methanol	395.32	37.5	-151.8	2216.7	2244.0	-	-	55-179
	$C_{19}H_{13}N_3O_6$	Tris(nitrophenyl)methane	379.32	38.5	-162.4	2271.5	2244.3	-	-	55-179
	$C_6H_5N_3O_5$	2-Amino-4,6-dinitrophenol	199.12	9.5	- 76.3	676.9	677.4	-	-	110
136	$C_7H_3F_3N_2O_4$	α,α,α-Trifluoro-3,5-dinitrotoluene	236.11	10.5	- 67.8	590.[illegible]	7[illegible].2	-	-	138
13	$C_6H_5N_3O_4$	2,4-Dinitroaniline	183.12	10.5	- 91.7	713.[illegible]	726.8	-	-	110
84	$C_7H_6N_2O_4$	2,4-Dinitrotoluene	182.13	13.0	-114.2	853.5	852.5	-	-	39
"	"	2,4- "	"	"	"	851.5	"	-	-	143
	"	2,3-Dinitrotoluene	"	"	"	870.2	"	-	-	39
	"	2,5-Dinitrotoluene	"	"	"	855.8	"	-	-	39
390	"	2,6-Dinitrotoluene	"	"	"	854.9	"	-	-	39
"	"	2,6- "	"	"	"	852.1	"	-	-	8
	"	3,4- "	"	"	"	8[illegible].6	"	-	-	39
	"	3,5- "	"	"	"	853.7	"	-	-	39
444	$C_9H_{10}N_2O_4$	Dinitromesitylene	210.19	19.0	-144.6	1175.7	1161.3	-	-	55-243
606	$C_{10}H_{14}N_4O_6$	N-[2-(2,4-Dinitroanilino)-ethyl]ethanolamine	270.24	22.0	-130.3	1342.8*	1360.7	-	-	55
340	$C_6H_3N_3O_8$	2,4,6-Trinitroresorcinol	245.11	5.5	- 35.[illegible]	[illegible]	[illegible].9	-	-	143
"	"	2,4,6- "	"	"	"	547.0	"	-	-	110
216	$C_6H_3N_3O_7$	2,4,6-Trinitrophenol	229.11	6.5	- 45.4	617.5	613.8	-	-	143
"	"	2,4,6- "	"	"	"	621.6	"	-	-	39
"	"	2,4,6- "	"	"	"	610.8	"	-	-	117
478	$C_6H_3N_3O_6$	1,3,5-Trinitrobenzene	213.11	7.5	- 56.3	663.8	660.3	-	-	39
"	"	1,3,5- "	"	"	"	675.1	"	-	-	119
273	"	1,2,4-Trinitrobenzene	"	"	"	674.0	"	-	-	39
270	$C_6H_4N_4O_6$	2,4,6-Trinitroaniline	228.12	9.0	- 56.1	673.2	669.9	-	-	110
277	$C_7H_5N_3O_7$	2,4,6-Trinitro-m-cresol	243.13	9.5	- 62.5	779.5	760.2	-	-	143
271	$C_7H_5N_3O_7$	2,4,6-Trinitroanisole	"	"	"	742.[illegible]	774.2	-	-	10
"	"	2,4,6- "	"	"	"	7[illegible].9	"	-	-	143
"	"	2,4,6- "	"	"	"	792.[illegible]	"	-	-	23
313	$C_7H_5N_3O_6$	2,4,6-Trinitrotoluene	227.13	10.[illegible]	- 74.0	821.0	815.6	-	-	39
"	"	2,4,6- "	"	"	"	836.4	"	-	-	117
314	"	2,3,4-Trinitrotoluene	"	"	"	831.3	"	-	-	39
410	"	2,3,5-Trinitrotoluene	"	"	"	824.2	"	-	-	39
411	"	2,3,6-Trinitrotoluene	"	"	"	825.8	"	-	-	39
413	"	3,4,5-Trinitrotoluene	"	"	"	823.5	"	-	-	39
412	"	3,4,6-Trinitrotoluene	"	"	"	826.0	"	-	-	39
376	$C_9H_5N_3O_7$	2-Propynyl picrate	267.15	13.5	"	1052.2	1023.0	-	-	71
208	$C_6H_2N_6O_{10}$	2,3,4,5,6-Pentanitroaniline	318.12	3.0	- 15.1	662.4	615.[illegible]	-	-	71

*Ref. 55 gives 1292.5 kcal/mole and a mol. wt. of [illegible]. Since the latter is incorrect the heat of combustion was recalculated from the value given, using the proper mol. wt.

TABLE 125

[illegible] TRINITROS ([illegible])

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^P, KCAL/MOLE OBSERVED	Q_c^P, KCAL/MOLE CALCULATED	Y'	X'	REF.
327	CHN_3O_6	Trinitromethane (Nitroform)	151.04	-1.5	+ 37.1	102.6	116.9	193.2	-1.5	44
"	"	"	"	"	"	117.5	"	113.1	-3.5	33
"	"	"	"	"	"	122.2	"	126.5	-1.5	71
	$C_5H_5N_3O_8$	1,1,1-Trinitroethanol acrylate	235.11	+4.5	- 30.6	564.1	562.3	51[illegible]	+4.5	1[illegible]
578	$C_5H_7N_3O_8$	Methyl 4,4,4-trinitrobutyrate	237.13	5.5	- 37.1	[illegible]	6[illegible]	579.1	5.5	128-1
579	"	1,1,1-Trinitro-2-propanol acetate	"	"	- 37.1	5[illegible]	546.8	56[illegible]	5.5	128-1
	$C_6H_7N_3O_8$	Vinyl 4,4,4-trinitrobutyrate	249.14	[illegible]	- 45.2	726.5	710.1	693.7	7.5	128-2
620	$C_6H_9N_3O_8$	Ethyl 4,4,4-trinitrobutyrate	251.16	8.5	- 54.1	761.6	755.0	733.4	8.5	128-1
646	$C_8H_{13}N_3O_8$	n-Butyl 4,4,4-trinitrobutyrate	279.21	14.5	- 83.1	1076.1	1064.7	1063.3	14.5	128-1
655	$C_{11}H_{20}N_4O_8$	2,3,3,4,5-Pentamethyl-1,1,1,5-[illegible]nitrohexane	336.30	24.0	-114.2	1631.5	1634.4	[illegible]46.5	24.0	129-1
		$y' = 292.59 + 52.37x'$						$\Sigma x' = 57.5$ $\Sigma y' = 6641.0$ $\Sigma x'y' = 71,459.75$ $\Sigma x'^2 = 1032.25$ $n = 10$		
210	CN_4O_8	Tetranitromethane	196.04	-6.0	+ 49.0	104.5	74.7	-	-	116
"	"	"	"	"	"	107.1	"	-	-	83

TABLE 126

ALIPHATIC C-N TRINITROS ([illegible])

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^P, KCAL/MOLE OBSERVED	Q_c^P, KCAL/MOLE CALCULATED	Y'	X'	REF.
310	$C_2H_3N_3O_7$	2,2,2-Trinitroethanol	181.07	1.5	+ 13.[illegible]	227.4	2[illegible]	212.[illegible]	-1.5	129-2
"	"	"	"	"	"	231.2	"	214.2	-1.5	71
567	$C_2H_3N_3O_6$	1,1,1-Trinitroethane	165.07	-0.5	+ 4.8	263.2	26[illegible]	257.5	-0.5	128-1
576	$C_3H_4N_4O_8$	1,1,1,3-Tetranitropropane	224.09	0.0	0.0	380.2	356.7	381.7	0.0	128-2
639	$C_4H_6N_4O_7$	4,4,4-Trinitrobutyramide	222.12	+4.0	- 28.8	477.6	47[illegible].9	476.1	+4.0	128-1
577	$C_5H_7N_3O_7$	5,5,5-Trinitro-2-pentanone	221.13	6.5	- 47.[illegible]	634.5	634.6	624.[illegible]	6.5	128-1
656	$C_6H_7N_3O_8$	2,2,2-Trinitroethanol methacrylate	249.14	7.5	- 48.2	7[illegible]7.8	707.7	[illegible]7.5	7.5	128-2
523	$C_5H_5N_7O_{14}$	1,1,1,3,5,5,5-Heptanitropentane	387.14	-1.5	+ 6.2	595.5	57[illegible]	259.5	-0.75	128-2
331	$C_5H_6N_8O_{13}$	1,3-Bis(2,2,2-trinitroethyl)-urea	386.16	0.0	0.0	592.[illegible]	[illegible]8.9	[illegible]	[illegible]	71
340	$C_6H_6N_6O_{14}$	2,2,2-Trinitroethanol 4,4,4-trinitrobutyrate	386.16	1.0	- 4.1	656.1	[illegible]	[illegible]7.5	0.5	71
586	$C_6H_7N_7O_{13}$	N-(2,2,2-Trinitroethyl)-4,4,4-trinitrobutyramide	385.17	2.5	- 10.4	726.2	721.0	35[illegible]	1.25	128-1
		$y' = 229.15 + 31.76x'$						$\Sigma x' = 15.9$ $\Sigma y' = 3971.9$ $\Sigma x'y' = 10,761.75$ $\Sigma x'^2 = 121.625$ $n = 11$		
266	$C_2N_4O_6$	Trinitroacetonitrile	176.05	+2.0	+ 18.2	230.1	17[illegible]	-	-	71
567	$C_2H_3N_3O_6$	1,1,1-Trinitroethane	165.07	+0.5	+ 4.8	291.1	2[illegible]	-	-	1[illegible]
562	$C_7H_{11}N_3O_7$	4,4-Dimethyl-5,5,5-trinitro-2-pentanone	217.15	+12.5	- 92.[illegible]	973.5	9[illegible]	-	-	129-1
683	$C_9H_{[illegible]}N_3O_{[illegible]}$	Diethyl(2,2,2-trinitroethyl)-malonate	323.22	14.5	- 71.6	1162.[illegible]	1[illegible]	-	-	129-1
331	$C_5H_6N_8O_{13}$	1,3-Bis(2,2,2-trinitroethyl)-urea	386.16	0.0	0.0	611.[illegible]	60[illegible].9	-	-	128-1
551	$C_7H_6N_8O_{13}$	1,3-Bis(2,2,2-trinitroethyl)-2-imidazolidone	[illegible]	2.0	- 17.[illegible]	[illegible]	[illegible]	-	-	128-1
584	$C_{10}H_{[illegible]}N_{[illegible]}O_{14}$	N,N'-Bis(2,2,2-trinitroethyl)-1,4-piperazinedicarboxamide	[illegible]	11.[illegible]	- 41.7	[illegible]	1272.5	-		128-1

TABLE 127

NITRATES (liquid)

ADL NO	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^v, KCAL/MOLE OBSERVED	Q_c^v, KCAL/MOLE CALCULATED	Y'	X'	REF.
667	$C_6H_{11}NO_7$	Dimethyl 3-hydroxyglutarate nitrate	2?0.22	18.5	-115.8	1127.1	1126.2	1097.0	18.5	128-1
9d	$C_2H_4N_2O_6$	1,2-Ethanediol dinitrate	152.07	0.0	0.0	266.5	264.5	130.4	0.0	153
37	$C_4H_8N_2O_7$	Diethylene glycol dinitrate	196.12	5.0	-40.8	547.3	541.9	263.0	2.5	109
"	"	"	"	"	"	547.6	"	263.2	2.5	95
635	$C_4H_8N_2O_6$	1,4-Butanediol dinitrate	180.12	6.0	-53.3	573.6	575.6	284.0	3.0	128-1
15	"	1,3-Butanediol dinitrate	"	"	"	574.3	"	294.3	3.0	128-1
642	"	1,2-Butanediol dinitrate	"	"	"	587.6	"	291.0	3.0	128-1
467	"	2,3-Butanediol dinitrate	"	"	"	574.8	"	294.6	3.0	128-1
632	$C_5H_{10}N_2O_6$	1,5-Pentanediol dinitrate	194.15	9.0	-74.2	732.6	735.6	363.5	4.5	128-1
		~~2,4-Pentanediol dinitrate~~	"	"	"	725.8	"	350.1	4.5	128-1
773	$C_6H_{12}N_2O_8$	Triethylene glycol dinitrate	240.17	10.0	-66.6	835.4	819.2	399.3	5.0	95
	"	"	"	"	"	837.1	-	392.7	5.0	93
634	$C_6H_{12}N_2O_6$	1,6-Hexanediol dinitrate	208.17	12.0	-92.2	870.1	892.5	436.2	6.0	128-1
972	$C_6H_{10}N_2O_{10}$	Diethyl tartrate dinitrate	296.17	"	-64.8	937.6	920.0	442.4	6.0	95
191	$C_3H_5N_3O_9$	Nitroglycerin	227.09	-0.5	+3.5	362.2	357.6	118.5	-0.167	95
"	"	"	"	"	"	363.8	"	117.4	-0.167	11?
"	"	"	"	"	"	365.5	"	120.0	-0.167	23
"	"	"	"	"	"	363.5	"	120.9	-0.167	106
"	"	"	"	"	"	365.5	"	119.7	-0.167	122
"	"	"	"	"	"	355.5	"	119.2	-0.167	36
"	"	"	"	"	"	357.2	"	122.4	-0.167	93
165	$C_4H_7N_3O_9$	1,2,3-Butanetriol trinitrate	241.12	+2.5	-16.6	517.5	524.7	170.6	+0.833	95
327	"	1,2,4-Butanetriol trinitrate	"	"	"	520.2	"	171.5	0.833	6
"	"	"	"	"	"	517.7	"	170.6	0.833	95
167	"	2-Methyl-1,2,3-propanetriol trinitrate	"	"	"	517.5	"	171.8	0.833	95
137	$C_5H_9N_3O_{10}$	3-(2-Hydroxyethoxy)-1,2-propanediol trinitrate	271.15	4.5	-26.6	650.9	645.1	209.5	1.5	95
"	"	"	"	"	"	654.9	"	211.5	1.5	128-1
645	$C_5H_9N_3O_9$	1,3,5-Pentanetriol trinitrate	255.15	5.[illegible]	-31.[illegible]	670.7	661.8	221.7	1.833	128-1
263	$C_5H_9N_3O_9$	2-Hydroxymethyl-2-methyl-1,3-propanediol trinitrate	"	"	"	671.9	676.3	223.1	1.833	23
1[illegible]	$C_6H_9N_4O_{11}$	1-Monolactin trinitrate	299.16	"	-29.4	715.2	695.6	232.5	1.833	93
626	[illegible]	2-(Allyloxymethyl)-2-(hydroxymethyl)-1,3-propanediol	311.21	12.5	-64.3	1067.7	1075.[illegible]	344.[illegible]	4.167	128-1
626	$C_8H_{15}N_3O_{10}$	2-(Hydroxymethyl)-2-(propoxymethyl)-1,3-propanediol	313.2?	1?.?	-69.?	1107.2	1114.1	362.7	4.5	6
237	$C_6H_{10}N_4O_{13}$	3,3'-Oxydi-1,2-propanediol tetranitrate	346.17	4.0	-1[illegible]	752.1	746.5	1[illegible].7	1.0	95
		$y' = 129.39 + 52.35x'$						$\Sigma x' = 86.829$ $\Sigma y' = 8816.1$ $\Sigma x'y' = 43,144.2305$ $\Sigma x'^2 = 609.414335$ $n = 33$		
150	$C_2H_4N_2O_5$	2-Nitroethanol nitrate	136.07	1.0	-[illegible]	2?0.1	275.[illegible]	-	-	95
102	$C_2H_5NO_3$	Ethyl nitrate (gas)	91.07	3.5	-61.5	324.4	-	-	-	16
"	"	"	"	"	"	322.4	-	-	-	35-223
"	"	" (liq)	"	"	"	-	3[illegible]	-	-	
673	$C_6H_{11}N_3O_9$	1,2,6-Hexanetriol trinitrate	271.19	9.?	-?6.?	816.4	814.4	-	-	128-1
	$C_8H_{13}N_3O_{10}$	Allylpentaerythritol trinitrate polymer	311.21	12.5	-61.[illegible]	934.8	1041.7	-	-	6
411	[illegible]	N-[illegible]yldiethanolamine dinitrate	[illegible]	13.0	-51.2	[illegible]	1225.3	-	-	[illegible]
627	$C_{11}H_{18}N_2O_8$	2,2-Bis(allyloxymethyl)-1,3-propanediol dinitrate	3?6.27	22.0	-114.9	1517.9	1476.1		-	128-1

TABLE 12?

NITRATES (cont'd)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_f, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
322	$(C_2H_3NO_3)_x$	Vinyl nitrate polymer	89.06	2.5	- 44.9	262.?	265.6	250.1	2.?	128-1
276	$C_7H_4N_4O_9$	2,4,6-Trinitrophenyl nitrate	288.13	7.0	- 44.4	7??.1	766.6	[illegible]	?.2	65
295	$C_8H_6N_4O_{10}$	2-(2,4,6-Trinitrophenoxy)-ethanol nitrate	318.16	9.0	- 50.3	[illegible]	[illegible]	[illegible]	9.5	124
610	[illegible]	1,2-Propanediol 2-nitrate 1-(5-nitrofuroate)	260.16	12.0	- 73.?	877.0	8??.2	756.5	12.0	65
168	$C_4H_7N_3O_8$	2-Methyl-2-nitro-1,3-propanediol dinitrate	225.12	3.5	- 24.9	531.?	533.8	212.2	1.75	80
41	$C_5H_{10}N_2O_6$	2,2-Dimethyl-1,3-propanediol dinitrate	194.15	9.0	- 74.2	715.9	711.3	3?6.?	?.5	66
74	$C_9H_7N_5O_{12}$	2-(3,5-Dinitrophenyl)-2-nitro-1,3-propanediol dinitrate	377.17	9.5	- 40.3	1022.7	1019.9	[illegible]	4.75	55
139	$C_9H_8N_4O_{10}$	2-Nitro-2-(m-nitrophenyl)-1,3-propanediol dinitrate	332.19	12.0	- 57.8	10??.?	1036.7	[illegible]	6.0	85
255	$C_6H_{11}N_3O_9$	2-Ethyl-2-(hydroxymethyl)-1,3-propanediol trinitrate	269.17	6.5	- 50.5	825.5	835.4	274.2	?.033	66
93	$C_4H_6N_4O_{12}$	Erythritol tetranitrate	302.11	-1.0	+ 5.3	4?3.3	466.9	114.4	-0.25	12?
"	"	"	"	"	"	451.4	"	111.0	-0.25	66
297	$C_5H_8N_4O_{12}$	Pentaerythritol tetranitrate	316.15	+2.0	- 10.1	616.4	620.8	153.6	+0.5	73
"	"	"	"	"	"	617.5	"	1??.8	0.5	73
"	"	"	"	"	"	616.9	"	150.7	0.5	143
231	$C_9H_{12}N_4O_{13}$	2,2,5,5-Tetrakis(hydroxymethyl)cyclopentanone tetranitrate	384.22	11.0	- 45.8	1077.4	1093.3	271.?	2.75	124
"	"	"	"	"	"	10?7.?	"	270.0	2.75	18?
229	$C_{10}H_{14}N_4O_{13}$	2,2,6,6-Tetrakis(hydroxymethyl)cyclohexanone tetranitrate	398.24	14.0	- 56.2	1232.7	1251.1	317.9	3.5	124
"	"	"	"	"	"	1210.7	"	309.?	3.5	66
623	$C_8H_{13}N_5O_{16}$	1-[2,2,2-Tris(hydroxymethyl)ethoxy]-1,2-propanediol pentanitrate	435.22	6.5	- 23.9	1014.0	1007.0	199.2	1.3	128-1
218	$C_8H_{16}N_6O_{15}$	Tetrakis(2-hydroxyethyl)ammonium pentanitrate	436.26	9.0	- 33.0	1116.6	1128.6	224.7	1.8	71
230	$C_9H_{13}N_5O_{16}$	2-Hydroxy-1,1,3,3-cyclopentanetetramethanol pentanitrate	431.23	9.5	- 35.2	1126.5	1116.0	223.?	1.9	124
228	$C_{10}H_{15}N_5O_{16}$	2-Hydroxy-1,1,3,3-cyclohexanetetramethanol pentanitrate	445.26	12.5	- 44.9	12??.9	1297.9	259.7	2.5	124
92	$C_6H_8N_6O_{18}$	Dulcitol hexanitrate	452.17	-2.0	+ 7.1	670.9	670.9	110.9	-0.333	65
433	"	Sorbitol hexanitrate	"	"	"	6??.5	"	1?4.5	-0.333	142
152	"	Mannitol hexanitrate	"	"	"	677.1	"	1??.?	-0.333	124
"	"	"	"	"	"	6??.9	"	112.7	-0.333	128-1
"	"	"	"	"	"	674.9	"	111.5	-0.333	65
"	"	"	"	"	"	7?1.7	"	115.0	-0.333	73
69	$C_{10}H_{16}N_6O_{19}$	Dipentaerythritol hexanitrate	5[illegible]	+9.0	- 27.?	12??.1	1262.1	208.8	+1.5	128
"	"	"	"	"	"	1250.7	"	206.1	1.5	66
2?9	$C_{12}H_{12}N_6O_{18}$	1,2,3,4,5,6-Benzenehexamethanol hexanitrate	528.26	12.0	- 36.3	1396.1	1395.7	233.7	2.0	71
		$y' = 128.41 + 52.51x'$						$\Sigma x' = 74.335$; $\Sigma y' = 7891.40$; $\Sigma x'y' = 32,465.5942$; $\Sigma x'^2 = 434.66623$; $n = 31.0$		
94	$C_2H_5N_3O_6$	Ethanolamine dinitrate	[illegible]	1.5	- 14.2	317.5	317.4	-	-	126
322	$(C_2H_3NO_3)_x$	Vinyl nitrate polymer	89.05	2.5	- 44.9	2?3.5	265.6	-	-	128-3
72	$C_8H_7N_3O_8$	2-(2,4-Dinitrophenoxy)-ethanol nitrate	273.16	11.5	- 67.4	941.6	925.3	-	-	124
608	$C_8H_7N_3O_8$	1-(o-Nitrophenyl)-1,2-ethanediol dinitrate	273.15	"	- 67.4	99?.9	945.7	-	-	65
645	$C_6H_{12}N_2O_6$	2,5-Hexanediol dinitrate	208.17	12.0	- 92.2	857.1	893.9	-	-	128-1
228	$C_{10}H_{15}N_5O_{16}$	2-Hydroxy-1,1,3,3-cyclohexanetetramethanol pentanitrate	445.26	12.5	- 44.9	1265.7	1297.9	-	-	66
433	$C_6H_8N_6O_{18}$	Sorbitol hexanitrate	452.17	-2.0	+ 7.1	723.?	670.9	-	-	128-1
69	$C_{10}H_{16}N_6O_{19}$	Dipentaerythritol hexanitrate	524.26	+9.0	- 27.5	117?.0	1262.1	-	-	93

TABLE 129

NITRAMINES (solid)

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^0, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
337	$C_4H_4N_8O_{14}$	Bis(2,2,2-trinitroethyl)-nitramine (BTNEN)	388.14	-4.0	+ 16.5	517.?	491.?	-?	-4.0	71
	$C_2H_4N_2O_2F_2$	2,2-Difluoroethylnitramine	126.07	3.0	- 38.1	287.5	303.6	239.9	3.0	71,8
35	$C_4H_8N_4O_8$	Diethanolnitramine dinitrate	240.14	4.0	- 26.7	571.7	559.3	291.3	4.0	86
202	$C_3H_7N_3O_5$	N-Methylethanolnitramine nitrate	165.11	4.5	- 43.6	473.8	487.5	319.6	4.5	66
593	$C_2H_6N_2O_2$	Ethylnitramine (liq)	90.08	5.0	- 88.8	372.9	370.9	353.?	5.0	136
327	$C_7H_4N_6O_{10}$	N-Methyl-N,2,3,4,6-pentanitroaniline	332.15	6.0	- 28.9	810.6	796.4	426.6	6.0	71
100	$C_{10}H_9N_8O_{17}$	2-(Hydroxymethyl)-2-(N,2,4,6-tetranitroanilino)-1,3-propanediol trinitrate	512.23	7.0	- 21.9	1160.7	1160.?	486.2	7.0	85
417	$C_6H_8N_4O_2$	(Nitroimino)diacetonitrile	140.10	8.0	- 91.4	566.5	561.5	533.4	8.0	128-3
307	$C_8H_6N_6O_{11}$	2-(N,2,4,6-Tetranitroanilino)ethanol nitrate	362.15	•	- 15.3	935.9	936.?	517.4	8.0	86
253	$C_7H_5N_5O_8$	Tetryl(N-methyl-N,2,4,6-tetranitroaniline)	287.15	8.5	- 47.4	833.9	831.6	557.2	8.5	143
•	•	•	•	•	•	836.4	•	549.7	8.5	23
•	•	•	•	•	•	836.8	•	551.1	8.5	23
•	•	•	•	•	•	836.5	•	549.8	8.5	110
•	•	•	•	•	•	841.4	•	554.7	8.5	39
•	•	•	•	•	•	836.5	•	551.3	8.5	86
240	$C_8H_7N_5O_8$	N-Methyl-N,2,4,6-tetranitro-m-toluidine	301.18	11.5	- 61.1	1009.8	996.1	727.2	11.5	39
305	$C_{10}H_{10}N_6O_{11}$	2-(N,2,4,6-Tetranitroanilino)-1-butanol nitrate	390.23	14.0	- 57.4	1259.6	1253.3	833.1	14.0	85
596	$C_6H_8N_4O_2$	3,3'-(Nitroimino)dipropionitrile	168.16	•	-133.2	863.2	860.9	819.0	14.0	128-3
325	$CH_4N_4O_4$	Methylenedinitramine (MEDINA)	136.07	0.0	0.0	219.5	230.3	+89.9	0.0	71
96	$C_2H_6N_4O_4$	Ethylenedinitramine (EDNA)	150.10	3.0	- 32.0	370.3	386.7	166.4	1.5	91
•	•	•	•	•	•	359.7	•	156.1	1.5	85
594	$C_3H_6N_4O_4$	1,3-Dinitroimidazolidine	162.11	5.0	- 49.3	487.1	496.7	222.7	2.5	128-3
	$C_5H_{11}N_5O_7$	1,3-Di(methylnitramino)-2-propanol nitrate	253.18	8.5	- 53.7	[illegible]	813.?	319.5	4.25	128-1
665	$C_{10}H_{14}N_6O_4$	2,7-Dimethyl-3,6-dinitro-3,6-diazaoctane-2,7-dicarbonitrile	284.28	24.0	-135.1	1490.5	1526.3	713.1	12.0	128-3
23	$C_3H_6N_6O_6$	RDX (Hexahydro-1,3,5-trinitro-s-triazine	222.13	3.0	- 21.6	506.2	504.7	149.7	1.0	143
•	•	•	•	•	•	504.3	•	148.0	1.0	23
•	•	•	•	•	•	504.0	•	157.7	1.0	23
•	•	•	•	•	•	501.8	•	147.2	1.0	81
•	•	•	•	•	•	503.8	•	147.3	1.0	54
984	$C_{12}H_{16}N_8O_{14}$	2,4,6-Tris(methylnitramino-methyl)-3,5-dinitrophenol	128.41	21.0	- 74.9	1601.7	1621.2	659.0	7.0	95
664	$C_{14}H_{20}N_8O_6$	2,10-Dimethyl-3,6,9-trinitro-3,6,9-triazaundecane-2,10-dicarbonitrile	372.34	28.0	-120.3	1863.9	1849.5	593.6	9.33	128-1
22	$C_4H_8N_8O_8$	HMX (Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	296.17	4.0	- 21.6	666.9	671.3	144.6	1.0	93
•	•	•	•	•	•	667.4	•	147.3	1.0	83
•	•	•	•	•	•	663.1	•	146.2	1.0	86

$$y' = 95.32 + 52.59x'$$

$\Sigma x' = 178.08$

$\Sigma y' = 12,659.5$

$\Sigma x'y' = 100,217.438$

$\Sigma x'^2 = 1,553.8614$

$n = 34$

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	OBSERVED	CALCULATED	Y'	X'	REF.
243	$C_7H_4N_6O_{10}$	N-Methyl-N,2,3,4,6-pentanitroaniline	332.15	6.0	- 28.9	843.?	796.4	-	-	113
•	•	•	•	•	•	829.?	•	-	-	71
253	$C_7H_5N_5O_8$	Tetryl	287.15	8.5	- 47.4	863.1	831.6	-	-	113
139	$C_{14}H_8N_{10}O_{12}$	N,N'-Dipicrylethylenedinitramine	472.??	16.0	- 44.7	1642.6	1608.4	-	-	85
763	$C_{14}H_{24}N_{10}O_8$	2,13-Dimethyl-3,6,9,12-tetranitro-3,6,9,12-tetrazatetradecane-2,13-dicarbonitrile	460.41	12.0	-111.2	2176.0	2175.0	-	-	128-3
[illegible]	$C_{18}H_{30}N_{12}O_{10}$	2,16-Dimethyl-3,6,9,12,15-pentanitro-3,6,9,12,15-pentazaheptadecane-2,16-dicarbonitrile	558.58	36.0	-105.?	2221.3	2501.2	-	-	128-3

TABLE 130

NITRAMIDES (cont'd)

ADL. NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	CALCULATED	Y'	X'	REF.
200	$CH_3N_3O_3$	Nitrourea	105.06	0.5	- 7.6	132.3	127.0	132.5	0.5	124
197	[illegible]$H_5N_3O_5$	N-Methyl-N-nitroglycolamide nitrate (MGAN)	179.09	2.5	- 22.3	378.2	382.9	227.3	2.5	86
"	"	"	"	"	"	331.0	"	230.1	2.5	85
144	$C_3H_3N_3O_4$	1-Nitrohydantoin	145.08	3.5	- 38.6	295.0	293.0	286.4	3.5	85
146	$C_4H_5N_3O_4$	5-Methyl-1-nitrohydantoin	159.10	6.5	- 65.4	446.0	445.4	445.1	6.5	85
56	$C_3H_4N_4O_5$	1,3-Dinitro-2-imidazolidone	176.09	3.0	- 27.3	390.6	396.6	176.6	1.5	126-3
"	"	"	"	"	"	385.9	"	174.2	1.5	66
"	"	"	"	"	"	388.9	"	175.7	1.5	85
63	$C_6H_8N_6O_{12}$	N,N'-Bis(2-hydroxyethyl)-N,N'-dinitrooxamide dinitrate (NENO)	356.17	4.0	- 18.0	716.2	708.3	210.0	2.0	124
"	"	"	"	"	"	707.9	"	205.6	2.0	35
"	"	"	"	"	"	710.3	"	206.8	2.0	85
51	$C_4H_4N_4O_6$	1,4-Dinitro-2,5-piperazinedione	204.10	"	- 31.4	452.8	448.4	208.0	2.0	85
58	$C_4H_6N_4O_6$	N,N'-Dimethyl-N,N'-dinitrooxamide	206.12	5.0	- 38.8	508.0	500.0	216.0	2.5	85
608	$C_4H_8N_6O_6$	1,1'-Ethylenebis(3-nitrourea)	236.15	6.0	- 40.7	550.4	550.6	298.1	3.0	85
53	$C_6H_8N_4O_6$	3,6-Dimethyl-1,4-dinitro-2,5-piperazinedione	232.16	10.0	- 68.9	759.1	755.7	364.8	5.0	85
607	$C_8H_{14}N_4O_8$	Diethyl ethylenebis(N-nitrocarbamate)	294.22	15.0	- 81.6	1035.4	1042.6	490.5	7.5	85
		$y' = 101.05 + 52.44x'$						$\Sigma x' = 45.00$ $\Sigma y' = 3027.7$ $\Sigma x'y' = 14,427.9$ $\Sigma x'^2 = 186.50$ $n = 16$		
	$C_2H_4N_4O_4$	Nitrobiuret	148.08	2.0	- 21.6	227.6	223.9	-	-	96
612	$C_6H_5N_3O_6$	N-Methyl-N,5-dinitro-2-furamide	215.12	8.5	- 63.2	768.0	673.6	-	-	85
	$C_2H_3N_5O_6$	Dinitrobiuret	193.08	-0.5	+ 4.1	203.3	200.0	-	-	96
55	$C_5H_6N_4O_6$	5,5-Dimethyl-1,3-dinitrohydantoin	218.13	7.0	- 51.3	604.2	578.5	-	-	85

TABLE 131

FLUORO (liquid)

ADL NO	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED (to HF)	OXYGEN BALANCE (to HF)	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	C_2H_5FO	2-Fluoroethanol	64.06	5.0	-124.9	289.9	289.0	275.3	5.0	138
	$C_4H_7FO_2$	Ethyl fluoroacetate	106.10	9.0	-135.7	502.7	503.1	484.7	9.0	138
	"	2-Fluoroethanol acetate	"	"	"	509.4	"	491.4	9.0	138
	C_6H_5FO	o-Fluorophenol	112.10	13.0	-185.5	706.6	695.6	705.9	13.0	138
	"	m-Fluorophenol	"	"	"	696.4	"	696.7	13.0	138
	C_5H_9FO	Ethyl 2-fluoro-2-propenyl ether	104.12	"	-199.8	731.3	731.4	695.3	13.0	138
	C_6H_5F	Fluorobenzene	96.10	14.0	-233.1	747.0	745.2	750.4	14.0	138
	C_6H_6FN	o-Fluoroaniline	111.12	14.5	-208.8	778.1	777.8	775.2	14.5	138
	"	m-Fluoroaniline	"	"	"	776.9	"	774.0	14.5	138
	"	p-Fluoroaniline	"	"	"	782.1	"	779.2	14.5	138
	C_7H_7F	o-Fluorotoluene	110.13	17.0	-247.0	903.2	903.4	906.4	17.0	138
	"	p-Fluorotoluene	"	"	"	903.0	"	906.2	17.0	138
	C_8H_9FO	m-Fluorophenetole	140.16	19.0	-216.9	1020.1	1024.8	1007.3	19.0	138
	"	p-Fluorophenetole	"	"	"	1023.3	"	1010.5	19.0	138
	$C_7H_{15}F$	1-Fluoro-n-heptane	118.19	21.0	-284.3	1121.4	1117.4	1121.4	21.0	138
	$C_8H_{17}F$	1-Fluoro-n-octane	132.16	24.0	-290.6	1270.0	1275.5	1275.8	24.0	138
	$C_2H_2F_2O_2$	Difluoroacetic acid	96.04	2.0	-33.3	133.4	128.2	66.2	1.0	138
	$C_2H_4F_2O$	2,2 Difluoroethanol	82.05	4.0	-50.9	244.7	247.3	115.0	2.0	138
	$C_2H_5F_2N$	2,2-Difluoroethylamine	81.07	5.5	-108.5	324.8	330.2	151.1	2.75	138
	$C_4H_6F_2O_2$	Ethyl difluoroacetate	124.09	8.0	-103.2	461.4	461.8	221.5	4.0	138
	"	2,2-Difluoroethyl acetate	"	"	"	454.6	"	218.1	4.0	138
	$C_6H_4F_2$	p-Difluorobenzene	114.09	13.0	-182.3	705.2	697.6	357.2	6.5	138
	$C_7H_6F_2$	ω,ω-Difluorotoluene	128.12	16.0	-199.8	855.2	[illegible]	429.3	8.0	138
	$C_4H_7F_4N$	Bis(2,2-difluoroethyl)amine	145.10	9.5	-104.8	562.3	566.8	135.0	2.375	138

$y' = 10.91 + 52.69x'$

$\Sigma x' = 267.125$
$\Sigma y' = 14,336.6$
$\Sigma x'y' = 213,371.353$
$\Sigma x'^2 = 3754.203125$
$n = 24$

TABLE 132

FLUORO (solid)

ADL NO	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED (to HF)	OXYGEN BALANCE (to HF)	Q_c^p, KCAL/MOLE OBSERVED	Q_c^p, KCAL/MOLE CALCULATED	Y'	X'	REF.
	$C_2H_3FO_2$	Fluoroacetic acid	78.02	3.0	-61.5	170.3	172.2	169.1	3.0	138
	C_2H_4FNO	2-Fluoroacetamide	77.06	4.5	-93.4	249.1	246.7	251.8	4.5	138
	C_6H_5FO	p-Fluorophenol	112.10	13.0	-185.5	696.5	695.6	696.5	13.0	138
	$C_7H_5FO_2$	o-Fluorobenzoic acid	140.11	14.0	-159.9	739.9	735.9	747.0	14.0	138
	"	m-Fluorobenzoic acid	"	"	"	737.4	"	[illegible]	14.0	138
	"	p-Fluorobenzoic acid	"	"	"	739.4	"	755.5	14.0	138
	C_8H_8FNO	m-Fluoroacetanilide	153.15	18.5	-151.3	977.7	977.9	981.0	18.5	138
	"	p-Fluoroacetanilide	"	"	"	978.5	"	951.5	18.5	138
	$C_9H_7FO_2$	o-Fluorocinnamic acid	166.15	19.0	-183.0	1013.5	1014.9	1005.9	19.0	138
	$C_9H_9FO_2$	Ethyl p-fluorobenzoate	168.16	20.0	-190.3	1050.2	1064.3	1035.5	20.0	138
	$C_{10}H_9FO_2$	Methyl m-fluorocinnamate	180.17	22.0	-195.4	1187.5	1182.1	1169.5	22.0	138
	$C_9H_{11}F$	Fluoropseudocumene	138.18	23.0	-276.3	1206.6	1212.0	1213.0	23.0	138
	$C_2H_3F_2NO$	2,2-Difluoroacetamide	95.05	3.5	-58.9	206.9	212.9	102.7	1.75	138
	$C_8H_7F_2NO$	2,2-Difluoroacetanilide	171.14	17.5	-163.6	944.4	939.8	473.9	8.75	138

$y' = 14.39 + 52.27x'$

$\Sigma x' = 194.0$
$\Sigma y' = 10,337.0$
$\Sigma x'y' = 176,119.05$
$\Sigma x'^2 = 3324.375$
$n = 14$

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TABLE 133

[illegible] (liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED (to HF)	OXYGEN BALANCE (to HF)	Q_c^o, KCAL/MOLE OBSERVED	Q_c^o, KCAL/MOLE CALCULATED	Y'	X'	REF
	$C_7H_5F_3O$	α,α,α-Trifluoro-m-cresol	162.11	15.0	[illegible]	761.9	754.6	762.4	16.0	[illegible]
	$C_7H_5F_3$	α,α,α-Trifluorotoluene	146.11	15.[illegible]	-164.3	809.[illegible]	807.3	812.[illegible]	15.0	[illegible]
	$C_8H_5F_3O_2$	α,α,α-Trifluoro-m-toluic acid (s)	190.12	"	-126.2	805.[illegible]	801.4	811.[illegible]	15.0	139
	$C_7H_6F_3N$	α,α,α-Trifluoro-m-toluidine	161.13	15.[illegible]	[illegible].9	829.[illegible]	835.7	[illegible]	15.[illegible]	135
	$C_9H_8F_3NO$	α,α,α-Trifluoro-m-acetotoluide (s)	203.15	19.5	-151.5	1041.[illegible]	1037.9	[illegible]	17.5	133
		$y' = 36.07 + 51.64x'$						$\Sigma x' = 79.0$ $\Sigma y' = 4259.7$ $\Sigma x'y' = 65{,}251.35$ $\Sigma x'^2 = 1256.5$ $n = 5$		

TABLE 134

NITROSAMINES (solid and liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c^o, KCAL/MOLE OBSERVED	Q_c^o, KCAL/MOLE CALCULATED	Y'	X'	REF.
195	$C_2H_6N_2O$	Dimethylnitrosamine (liq)	74.08	6.0	-129.6	394.3	378.1	371.[illegible]	6.0	190
675	$C_8H_{10}N_2O$	N-Ethyl-N-nitrosoaniline (s)	[illegible]	20.0	-213.1	1118.[illegible]	1068.9	1142.2	20.0	190
676	$C_{12}H_{10}N_2O$	Diphenylnitrosamine (s)	198.22	28.0	-226.0	2514.3	1516.1	[illegible]	28.0	[illegible]
"	"	"	"	"	"	1530.[illegible]	"	1532.4	28.0	213
776	$C_5H_{10}N_6O_2$	3,7-Dinitroso-1,3,5,7-tetraazabicyclo$\boxed{3.3.1}$nonane (s)	186.18	13.0	-111.7	[illegible]	[illegible]	391.4	6.5	[illegible]
"	"	"		"	"	873.1	"	395.2	6.5	207
24	$C_3H_6N_6O_3$	Hexahydro-1,3,5-trinitroso-s-triazine (R-Salt) (s)	174.13	6.0	-55.1	553.5	516.9	164.5	2.0	201
"	"	"	"	"	"	566.2	"	165.[illegible]	2.0	15,197
"	"	"	"	"	"	559.1	"	166.4	2.0	207
		$y' = 56.03 + 53.13x'$						$\Sigma x' = 101.0$ $\Sigma y' = 5870.4$ $\Sigma x'y' = 117{,}255.90$ $\Sigma x'^2 = 2160.5$ $n = 9$		
195	$C_2H_6N_2O$	Dimethylnitrosamine (liq)	74.08	6.0	-129.6	[illegible]0.3[a]	393.1	-	-	190

[a] This value as reported by Chem. Abstr. is obviously a misprint.

TABLE 135

THIOPHENES (solid and liquid)

ADL NO.	FORMULA	NAME	MOL. WT.	OXYGEN* REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	Q_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
[illegible]	$C_4H_2N_2O_4S$	2,4-Dinitrothiophene (s)	174.13	7.0	-64.3	563.1	533.2	395.6	7.0	60
519	$C_4H_3NO_2S$	2-Nitrothiophene (s)	129.13	9.5	-117.7	616.7	617.7	520.6	9.5	60
521	$C_5H_4N_2O_4S$	3-Methyl-2,5-dinitrothiophene (s)	188.16	10.0	-85.0	737.1	735.2	571.0	10.0	60
522	C_4H_4S	Thiophene (liq)	84.13	12.0	-228.2	667.2	663.7	661.7	12.0	77
"	"	"	"	"	"	664.3	"	656.6	12.0	53
520	$C_5H_5NO_2S$	3-Methyl-2-nitrothiophene (s)	143.16	12.5	-134.7	777.2	777.7	686.3	12.5	60
		$y' = 21.59 + 53.08x'$						$\Sigma x' = 63.0$ $\Sigma y' = 3671.3$ $\Sigma x'y' = 37,421.25$ $\Sigma x'^2 = 693.5$ $n = 6$		
699	C_4H_4S	Thiophene (liq)	84.13	12.0	-228.2	670.5	663.9	-		2-37
	$C_5H_4O_2S$	2-Thiophene carboxylic acid (s)	128.09	12.0	-112.7	616.2	600.0	-	-	2-135

*Calculated to SO_2

TABLE 136

NITROSO (solid)

ADL NO.	FORMULA	NAME	MOL. WT	OXYGEN REQUIRED	OXYGEN BALANCE	Q_c°, KCAL/MOLE OBSERVED	Q_c°, KCAL/MOLE CALCULATED	Y'	X'	REF.
811	$C_8H_{10}N_2O$	N,N-Dimethyl-p-nitrosoaniline	150.18	20	-213.1	1124.1	1123.2	1107.0	20	190, 2-212
"	"	"	"	"	"	1126.9	"	1106.5	20	211
	$C_{12}H_{10}N_2O$	p-Nitrosodiphenylamine	198.22	28	-226.0	1549.2	1537.6	1525.3	28	211
80	$C_6H_4N_2O_4$	Dinitrosoresorcinol	168.11	10	-95.2	582.5	559.1	267.6	5	190
		$y' = 20.8[illegible] + 54.01x'$						$\Sigma x' = 73.0$ $\Sigma y' = 4026.3$ $\Sigma x'y' = 84,424.40$ $\Sigma x'^2 = 1609.0$ $n = 4$		

TABLE 137
HEAT OF HYDRATION[a]

$$Q_{Hydration} = Q_{Formation\ of\ hydrate} - Q_{Formation\ of\ anhydrous\ salt} - Q_{Formation\ of\ water}$$

Hydrate	Q_F kcal/mole	Anhydrous Compound	Q_F kcal/mole	$\Delta Q_{F/H_2O}$ kcal/mole
$N_2H_4 \cdot H_2O$ (aq.)	63.9	N_2H_4 (aq.)	-8.2	72.1
$N_2H_4 \cdot H_2O$ (liq)	58.0	N_2H_4 (liq)	-12.1	70.1
$NaOH \cdot H_2O$ (s)	175.3	NaOH (s)	102.0	73.3
$H_4P_2O_7 \cdot 1.5H_2O$ (s)	637.5	$H_4P_2O_7$ (s)	513.7	82.4
$H_4P_2O_7 \cdot 1.5H_2O$ (liq)	634.4	$H_4P_2O_7$ (liq)	529.4	70.0
$H_2SO_4 \cdot H_2O$ (s)	273.3	H_2SO_4 (s)	196.3	76.9
$H_2SO_4 \cdot H_2O$ (liq)	268.7	H_2SO_4 (liq)	193.8	74.9
$H_2SeO_4 \cdot H_2O$ (s)	204.5	H_2SeO_4 (s)	130.3	74.2
$H_2SeO_4 \cdot H_2O$ (liq)	200.0	H_2SeO_4 (liq)	126.8	73.2
$(COOH)_2 \cdot 2H_2O$ (s)	340.2	$(COOH)_2$ (s)	197.6	71.3
$(COONH_4)_2 \cdot H_2O$ (s)	339.1	$(COONH_4)_2$ (s)	267.2	71.9
$(NH_4)_2SO_3 \cdot H_2O$ (s)	283.6	$(NH_4)_2SO_3$ (s)	212.3	71.3
$3PbI_2 \cdot PI_3 \cdot 12H_2O$ (s)	977.3	$3PbI_2 \cdot PI_3$ (s)	131.8	70.6
$3PbI_2 \cdot AsI_3 \cdot 12H_2O$ (s)	952.2	$3PbI_2 \cdot AsI_3$ (s)	111.0	70.1
$LiBr \cdot H_2O$ (s)	158.4	LiBr (s)	83.8	74.6
$LiBr \cdot 2H_2O$ (s)	230.0	LiBr (s)	83.8	73.1
$LiBr \cdot 3H_2O$ (s)	302.0	LiBr (s)	83.8	72.4
$Li_2SO_4 \cdot H_2O$ (c)	413.7	$LiSO_4$ (s)	342.35	71.2
$KF \cdot 2H_2O$ (s)	277.1	KF (s)	134.5	71.3
$KF \cdot 4H_2O$ (s)	418.0	KF (s)	134.5	70.9

$\Sigma(\Delta Q_F) = 1455.8$

$n = 20$

$Av. \Delta Q_F = 72.8$

$Q_{Hydration} = 72.8 - 68.3 = + 4.5$ kcal/mole

[a] Data from Ref. 16.

TABLE 130

SALT LINK

$$Q_c^p \text{ (salt link)} = Q_c^p \text{ (salt)} - Q_c^p \text{ (acid + base)} = -Q_f^p \text{ (salt)} + Q_f^p \text{ (acid + base)} - Q_f^p \text{ (salt)}$$

Formula	Name		Mol. wt.	Ox. Needed	Ox. Bal.	Heat Observed, kcal/mole Formation Q_f	Combustion Q_c^p	Q_c^p per salt link kcal/mole	Ref.
$CH_6N_2O_3$	Methylamine nitrate	(s)	94.07	2.0	- 34.0	-	218.4		29
CH_5N	Methylamine	(liq)	31.06	4.5	-231.8	-	254.1		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	41.4	-7.3		82a
								-28.4	
$C_2H_8N_2O_3$	Dimethylamine nitrate	(s)	108.10	5.0	- 74.0	-	352.4		29
C_2H_7N	Dimethylamine	(liq)	45.08	7.5	-266.2	-	413.7		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-24.6	
$C_3H_{10}N_2O_3$	Trimethylamine nitrate	(s)	122.13	8.0	-104.8	-	550.7		29
C_3H_9N	Trimethylamine	(liq)	59.11	10.5	-284.2	-	571.9		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-15.9	
$C_2H_8N_2O_3$	Ethylamine nitrate	(liq)	108.10	5.0	- 74.0	-	374.5		29
C_2H_7N	Ethylamine	(liq)	45.08	7.5	-266.2	-	407.2		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-26.1	
$C_4H_{12}N_2O_3$	Diethylamine nitrate	(s)	136.15	11.0	-129.3	-	657.4		29
$C_4H_{11}N$	Diethylamine	(liq)	73.14	13.5	-295.3	-	725.5		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-33.8	
$C_6H_{16}N_2O_3$	Triethylamine nitrate	(s)	164.20	17.0	-165.7	-	1013.6		29
$C_6H_{15}N$	Triethylamine	(liq)	101.19	19.5	-308.3	-	1043.[illegible]		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-22.4	
$C_6H_8N_2O_3$	Aniline nitrate	(s)	156.14	11.0	-113.2	-	707.9		153
"	"	(s)	"	"	"	-	775.1		29
C_6H_7N	Aniline	(liq)	93.12	15.5	-266.3	-	809.1		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-10.3 (av)	
$C_{13}H_{10}N_2O_3$	Acridine nitrate	(s)	242.23	28.0	-184.9	-	1553.3		153
$C_{13}H_9N$	Acridine	(liq)	179.21	30.5	-272.3	-	1577.6		2
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-17.2	
$C_{13}H_{11}N_3O_3$	2-Aminoacridine mononitrate	(s)	257.24	28.5	-177.3	-	1562.0		153
$C_{13}H_{10}N_2$	2-Aminoacridine	(s)	194.23	31.0	-255.4	-	1601.7		153
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-14.4	
$C_{13}H_{11}N_3O_3$	9-Aminoacridine mononitrate	(s)	257.24	28.5	-177.3	-	1593.7		153
$C_{13}H_{10}N_2$	9-Aminoacridine	(s)	194.23	31.0	-255.4	-	1601.9		153
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-30.9	
$C_{13}H_{12}N_4O_3$	3,6-Diaminoacridine mononitrate	(s)	272.26	29.0	-170.4	-	1594.5		153
$C_{13}H_{11}N_3$	3,6-Diaminoacridine	(s)	209.24	31.5	-240.9	-	1628.4		153
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-26.6	
$C_2H_{10}N_4O_6$	Ethylenediamine dinitrate	(s)	186.13	3.0	- 25.8	-	376.3		126
"	"		"	"	"	-	373.2		66
$C_2H_8N_2$	Ethylenediamine	(liq)	60.10	8.0	-213.0	-	451.3		calc.
HNO_3	Nitric acid x2	(liq)	63.02	-2.5	+ 63.5	-	-14.6		82a
								-31.3 (av)	
$C_2H_7N_3O_6$	Ethanolamine dinitrate	(s)	169.10	1.5	- 14.2	-	317.5		121
"	"		"	"	"	-	323.8		29
$C_2H_8N_2O_4$	Ethanolamine nitrate	(liq)	126.08	4.0	- 60.3	-	359.0		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-31.0 (av)	
$C_7H_{10}N_2O_3$	Benzylamine nitrate	(s)	170.17	16.0	-150.4	-	942.7		29
C_7H_9N	Benzylamine	(liq)	107.15	18.5	-276.2	-	961.1		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		82a
								-11.1	
$C_2H_6N_2O_5$	Glycine nitrate	(s)	138.08	2.0	- 23.2	-	219.5		29
$C_2H_5NO_2$	Glycine	(s)	75.07	4.5	- 95.9	126.3	234.[illegible]		67a
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		67c
								- 5.6	
$C_6H_{14}N_6O_6$	Hexamethylenetetramine dinitrate	(s)	226.21	13.0	- 91.7	-	943.4		36
"	"		"	"	"	-	957.5		33
"	"		"	"	"	-	952.3		35
$C_6H_{12}N_4$	Hexamethylenetetramine	(s)	140.19	18.0	-205.4	-	1005.1		23
"	"		"	"	"	-	1007.9		13
"	"		"	"	"	-	1004.7		32
HNO_3	Nitric acid (x2)	(liq)	63.02	-2.5	+ 63.5	-	-14.6		82a
								-19.2 (av)	

TABLE 13d (cont'd)

SALT LINK

Formula	Name		Mol. wt.	O_2 Needed	Ox. Bal.	Heat Observed, kcal/mole Formation Q_f	Combustion Q_c	Q_f per salt link kcal/mole	Ref.
$CH_5N_3O_4$	Urea nitrate	(s)	123.06	0.5	- 6.5	-	134.3		124
CH_4N_2O	Urea	(s)	60.06	3.0	-159.4	-	150.4		calc.
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	-	-7.3		62a
								- 6.6	
$CH_5N_3O_3S$	Thiourea nitrate	(s)	139.07	3.[illegible]	- 40.3	74.7	-		62a
CH_4N_2S	Thiourea	(s)	76.07	6.0	-126.2	22.1	-		62a
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	41.4	-		62a
								-11.0	
$H_4N_2O_4$	Hydroxylamine nitrate	(s)	96.05	-2.0	+ 33.3	86.9	-		16
H_3NO	Hydroxylamine	(s)	33.03	+0.5	- 24.2	25.5	-		62a
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	41.4	-		62a
								-20.0	
$H_4N_2O_3$	Ammonium nitrate	(s)	80.05	-1.0	+ 20.0	87.3	-		62a
H_3N	Ammonia	(liq)	17.03	+1.5	-140.9	16.0	-		62a
HNO_3	Nitric acid	(liq)	63.02	-2.5	+ 63.5	41.4	-		62a
								-27.3	
$H_5N_3O_3$	Hydrazine mononitrate	(aq)	95.07	-0.5	+ 8.4	58.4	-		73
H_4N_2	Hydrazine	(aq)	32.05	+2.0	- 99.8	-8.2	-		73
HNO_3	Nitric acid	(aq)	63.02	-2.5	+ 63.5	47.6	-		62a
								-13.2	
$H_6N_4O_6$	Hydrazine dinitrate	(aq)	158.09	-3.0	+ 30.4	103.4	-		73
H_4N_2	Hydrazine	(aq)	32.05	+2.0	- 99.8	-8.2	-		73
HNO_3	Nitric acid (x2)	(aq)	63.02	-2.5	+ 63.5	98.8	-		62a
								- 6.4	
$H_6N_2O_4S$	Hydrazine sulfate	(aq)	130.08	1.0	- 12.3	219.3	-		73
H_4N_2	Hydrazine	(aq)	32.05	2.0	- 99.8	-8.2	-		73
H_2SO_4	Sulfuric acid	(aq)	98.08	-1.0	+ 16.3	216.9	-		62a
								-10.6	
$H_{10}N_4O_4S$	Dihydrazine sulfate	(aq)	162.12	3.0	- 29.6	225.3	-		73
H_4N_2	Hydrazine (x2)	(aq)	32.05	2.0	- 99.8	-16.4	-		73
H_2SO_4	Sulfuric acid	(aq)	98.08	-1.0	+ 16.3	216.9	-		62a
								-12.7	
H_5N_2Cl	Hydrazine hydrochloride	(aq)	68.52	2.0	- 46.7	44.6	-		73
H_4N_2	Hydrazine	(aq)	32.05	2.0	- 99.8	-8.2	-		73
HCl	Hydrochloric acid	(aq)	36.47	0.0	0.0	40.0	-		62a
								-12.8	
$H_6N_2Cl_2$	Hydrazine dihydrochloride	(aq)	104.93	2.0	- 30.5	85.0	-		62a
H_4N_2	Hydrazine	(aq)	32.05	2.0	- 99.8	-8.2	-		73
HCl	Hydrochloric acid (x2)	(aq)	36.47	0.0	0.0	80.5	-		62a
								- 6.1	
CH_6NCl	Methylamine hydrochloride	(aq)	67.52	4.5	-106.6	-	-	-13.0	16
C_2H_8NCl	Dimethylamine hydrochloride	(aq)	81.55	7.5	-147.1	-	-	-11.8	16
C_2H_8NCl	Ethylamine hydrochloride	(s)	81.55	7.5	-147.1	-	-	- 3.4	16
$CH_6N_3^+$	Guanidine ion	(aq)	60.08	7.0	-166.4	-	-	-11.	16
$C_2H_6NO_2Cl$	Ammonium monochloroacetate	(aq)	111.53	4.5	- 64.5	-	-	-12.7	16
$C_2H_4NO_2Cl_3$	Ammonium trichloroacetate	(aq)	180.43	2.5	- 22.2	-	-	-13.1	16
$C_2H_5NO_4$	Ammonium hydrogen oxalate	(aq)	107.07	2.5	- 37.4	-	-	-12.5	16
$C_2H_7NO_3$	Ammonium glycolate	(aq)	93.08	4.5	- 77.4	-	-	-12.2	16
$C_2H_7NO_4$	Ammonium glyoxalate	(aq)	109.08	3.5	- 51.3	-	-	-12.2	16
CH_5NO_2	Ammonium formate	(aq)	63.06	2.5	- 63.4	-	-	-11.9	16
$C_2H_8N_2O_4$	Diammonium oxalate	(s)	124.10	4.0	- 51.6	267.2	-		16
H_3N	Ammonia (x2)	(liq)	17.03	1.5	-140.9	33.2	-		62a
$C_2H_2O_4$	Oxalic acid	(s)	90.04	1.0	- 17.8	206.2	60.2		calc.
								-11.7	
$C_6H_6N_4O_7$	Ammonium picrate	(s)	246.14	8.0	- 52.0	-	693.9		122
H_3N	Ammonia	(liq)	17.03	1.5	-140.9	-	97.0		62a
$C_6H_3N_3O_7$	Picric acid	(s)	229.11	6.5	- 45.4	-	613.4		calc.
								-17.4	
$CH_8N_2O_3$	Ammonium carbonate	(aq)	96.09	3.0	- 50.0	221.6	-		16
H_3N	Ammonia (x2)	(aq)	17.03	1.5	-140.9	33.6	-		62a
CH_2O_3	Carbonic acid	(aq)	62.03	0.0	0.0	+167.0	-		62a
								- 9.0	
$C_2H_7NO_3$	Methylamine hydrogen carbonate	(aq)	93.08	4.5	- 77.4	-	-	- 9.0	16

TABLE 130 (cont'd)

SALT LINK

Formula	Name		Mol. wt.	Ox. Needed	Ox. Bal.	Heat Observed, kcal/mole Formation Q_f^p	Combustion Q_c^p	Q_c^p salt link kcal/mole	Ref.
$C_2H_7NO_2$	Ammonium acetate	(s)	77.08	5.5	-114.2	149.0	272.2		16
H_3N	Ammonia	(liq)	17.03	1.5	-140.9	-	97.0		82a
$C_2H_4O_2$	Acetic acid	(liq)	60.06	4.0	-106.6	-	209.6		calc.
								-26.4	
CH_4N_2O	Ammonium cyanate	(aq)	60.06	3.0	- 79.9	68.5	-		82a
H_3N	Ammonia	(aq)	17.03	1.5	-140.9	19.3	-		82a
CHNO	Cyanic acid	(aq)	43.03	1.5	- 55.8	35.1	-		82a
								-14.1	
$CH_4N_4O_6$	Ammonium nitroform	(s)	168.07	-2.0	- 19.0	-	195		Pi[illegible]
H_3N	Ammonia	(liq)	17.03	[illegible]	-140.9	-	97.0		82a
CHN_3O_6	Nitroform	(liq)	151.04	-3.5	+ 37.1	-	114.9		calc.
								-10.[illegible]	
[illegible]	Ethylenediamine dinitroform	(s)	[illegible]	4.5	- 3[illegible].1	-	[illegible]		71
$C_2H_8N_2$	Ethylenediamine	(liq)	60.10	8.0	-213.3	-	451.[illegible]		calc.
CHN_3O_6	Nitroform (x2)	(liq)	151.04	-3.5	+ 37.1	-	22[illegible].0		calc.
								-11.4	
H_4N_4	Ammonium azide	(aq)	60.06	2.0	- 53.3	-25.9	-		16
H_3N	Ammonia	(aq)	17.03	1.5	-140.9	19.3	-		82a
HN_3	Hydrazoic acid	(aq)	43.03	0.5	- 18.6	-54.5	-		16
								- 5.3	
[illegible]	MEDINA dihydrazine salt	(s)	200.17	2.0	- 16.0	-	407.8		71
H_4N_2	Hydrazine (x2)	(liq)	32.05	2.0	- 9[illegible]	-	297.2		73
$CH_4N_4O_4$	MEDINA	(s)	136.07	0.0	0.0	-	244.3		calc.
								-19.9	
$C_8H_{11}N_2OCl$	p-Nitrosodimethylaniline hydrochloride	(s)	186.65	20.0	-171.4	-	1120.5		135
$C_8H_{10}N_2O$	p-Nitrosodimethylaniline	(s)	150.18	20.0	-213.1	-	1120.2		calc.
HCl	Hydrochloric acid	(liq)	36.47	0.0	0.0	-	26.0		82a
								-25.4	
CH_4N_2	Ammonium cyanide	(s)	44.06	4.0	-145.3	0.0	-		82a
H_3N	Ammonia	(liq)	17.03	1.5	-140.9	16.6	-		82a
CHN	Hydrocyanic acid	(liq)	27.03	2.5	-148.0	-25.2	-		82a
								- 6.5	
CH_5NO_3	Ammonium hydrogen carbonate	(aq)	79.06	1.5	- 30.4	196.9	-		82a
H_3N	Ammonia	(aq)	17.03	1.5	-140.9	19.3	-		82a
CH_2O_3	Carbonic acid	(aq)	62.03	0.0	0.0	167.0	-		82a
								-10.6	
CH_4N_2S	Ammonium thiocyanate	(aq)	76.07	6.0	-126.2	15.5	-		82a
H_3N	Ammonia	(aq)	17.03	1.5	-140.9	19.3	-		82a
CHNS	Thiocyanic acid	(aq)	59.04	4.5	-122.0	-17.7	-		82a
								-12.9	
H_4NOCl	Hydroxylamine monohydrochloride	(aq)	69.50	0.5	- 11.5	70.7	-		82a
H_3NO	Hydroxylamine	(aq)	33.03	0.5	- 24.2	21.7	-		82a
HCl	Hydrochloric acid	(aq)	36.47	0.0	0.0	40.0	-		82a
								- 9.0	

$\Sigma(\Delta Q)$ = -[illegible]3.2
n = 52
Av. Q_c^p = -16.1 kcal/mole

$C_{12}H_8N_8O_{12}$	Hexanitrodiphenylamine ammonium salt	(s)	456.25	16.0	- 56.1	-	1422.6	119
[illegible]	Oxalimidic dihydrazide dinitrate	(s)	179.15	5.5	- 49.1	-	443.5	126-1
$H_8N_2O_6S$	Hydroxylamine sulfate	(aq)	131.06	-0.5	+ 6.1	244.4	-	16
[illegible]	Hydroxylamine dihydrochloride	(aq)	105.96	-0.5	- 7.6	104.0	-	82a
$C_{12}H_{14}N_2I_2$	Benzidine dihydroiodide	(s)	440.09	30.0	-109.1	-	1577.0	99

CONFIDENTIAL

TABLE 139

LIST OF COMPOUNDS

C -

1. Acetylene
2. 1-(Aminoguanyl)-4-(nitroguanyl)-1-tetrazene
3. Ammonium nitrate
4. Nitroform, ammonium salt
5. Picric acid, ammonium salt
6. 4-Hydroxytetrahydropyran-3,3,5,5-tetramethanol pentanitrate
7. Dimethylazaurolic acid
8. Sodium azide
9. 2-Azidoethanol
10. 2-Azidoethanol nitrate
11. 5-Azido-1-hydroxy-1H-tetrazole
12. 3-Azido-1,2-propanediol dinitrate
13. 4,4'-Isopropylidenebis(2,6-dinitrophenol)
14. 4,4'-Sulfonylbis(2,6-dinitrophenol)
15. 1,3-Butanediol dinitrate
16. Ethylenediamine dichlorate
17. 2-Chloroethanol nitrate
18. 3-Hydroxypropionitrile nitrate
19. Glycolonitrile nitrate
20. Cyanuric triazide
21. Tetrahydro-3,5-dinitro-1,3,5,2H-oxadiazine
22. HMX
23. RDX
24. ~~Hexahydro-1,3,5-trinitroso-s-triazine~~
25. 2,4,6,8-Tetranitro-2,4,6,8-tetrazanonane-1,9-diol diacetate
26. 2,4,6-Trinitro-2,4,6-triazaheptane-1,7-diol diacetate
27. 5,5'-(Diazoamino)di-1H-tetrazole
28. 5,7-Dinitro-1,2,3-benzoxadiazole
29. Diazonium salts
30. 1,9-Dicarboxy-2,4,6,8-tetranitrophenazine N^{10}-oxide
31. α,α'-Azobis(N'-chloroformamidine)
32. 1,2-Dichloro-3,5-dinitrobenzene
33. Guanylurea perchlorate
34. N,N'-Bis(2,3-dihydroxypropyl)oxamide tetranitrate
35. Diethanolnitramine dinitrate
36. Diethanolnitrosamine dinitrate
37. Diethylene glycol dinitrate
38. N,N'-Dimethylethylenedinitramine
39. 2-(Methoxymethyl)-2-nitro-1,3-propanediol dinitrate
40. 2-Ethyl-2-nitro-1,3-propanediol dinitrate
41. 2,2-Dimethyl-1,3-propanediol dinitrate
42. 1,3-Dinitramino-2-propanol nitrate
43. 2,4-Dinitroaniline
44. 2,4-Dinitroanisole
45. m-Dinitrobenzene
46. 2,4-Dinitrobenzyl nitrate
47. 2,2-Dinitro-1-butanol
48. 1-Chloro-2,4-dinitrobenzene
49. 4,6-Dinitro-o-cresol
50. N,N'-Diethyl-N,N'-dinitrooxamide

TABLE 139 (cont'd)

C-

51. 1,4-Dinitro-2,5-piperazinedione
52. 2,3-Dimethyl-2,3-dinitrobutane
53. 3,6-Dimethyl-1,4-dinitro-2,5-piperazinedione
54. 3a,6a-Dimethyl-1,6-dinitroglycoluril
55. 5,5-Dimethyl-1,3-dinitrohydantoin
56. 4,6-Dinitro-m-xylene-α,α'-diol dinitrate
57. 2,5-Dinitro-p-xylene-α,α'-diol dinitrate
58. N,N'-Dimethyl-N,N'-dinitrooxamide
59. 2,2-Dimethyl-1,3-dinitropropane
60. N,N'-Dimethyl-N,N'-dinitrosulfamide
61. N,N'-Dimethyl-N,N'-dinitrotartramide dinitrate
62. 1,5-Dinitro-2,3-dinitrosobenzene
63. N,N'-Bis(2-hydroxyethyl)-N,N'-dinitrooxamide dinitrate
64. N,N'-Bis(2-hydroxyethyl)-N,N'-dinitrosulfamide dinitrate
65. 1,1-Dinitroethane
66. 1,3-Dinitro-2-imidazolidone
67. 2,5-Dinitrofuran
68. 1,6-Dinitroglycoluril
69. Tetrahydro-5-hydroxy-1,3-dinitro-2(1H)-pyrimidone nitrate
70. 2-Methyl-1,2-dinitropropane
71. 2,4-Dinitrophenol
72. 2-(2,4-Dinitrophenoxy)ethanol nitrate
73. α,3,5-Trinitrotoluene
74. 2-(3,5-Dinitrophenyl)-2-nitro-1,3-propanediol dinitrate
75. 1,4-Dinitropiperazine
76. 1,1-Dinitropropane
77. 2,2-Dinitro-1-propanol
78. 2,4-Dinitroresorcinol
79. N,N'-Dinitrosobenzamide
80. 2,4-Dinitrosoresorcinol
81. 2,5-Bis(hydroxymethyl)-2,5-dinitro-1,6-hexanediol tetranitrate
82. 2,6-Bis(hydroxymethyl)-2,6-dinitro-1,7-heptanediol tetranitrate
83. 1,10-Dinitro-1,4,7,10-tetrapicryl-1,4,7,10-tetrazadecane
84. 2,4-Dinitrotoluene
85. Diethanolamine trinitrate
86. 4,6-Dinitro-m-xylene
87. Oxydimethanol dinitrate
88. 2,4,6,8-Tetranitro-2,4,6,8-tetrazanonane-1,9-diol dinitrate
89. Dipentaerythritol hexanitrate
90. N,N'-Dipicryl-1,3-propanedinitramine
91. 3,7-Dinitro-1,3,5,7-tetrazabicyclo[3.3.1] nonane
92. Dulcitol hexanitrate
93. Erythritol tetranitrate
94. Ethanolamine dinitrate
95. Ethylenediamine dinitrate
96. Ethylenedinitramine
97. 1,2-Ethanediol dilactate dinitrate
98. 1,2-Ethanediol dinitrate
99. 1,2-Ethanediol glycolate dinitrate
100. 1,2-Ethanediol lactate dinitrate
101. 3,4-Bis(2-nitroethyl)-1,2,3,4-dioxadiazetidine
102. Ethyl nitrate
103. Galactan trinitrate
104. 1,3(or 2,3)-dichloro-2(or 1)-propanol nitrate

TABLE 139 (cont'd)

C-

105. Glycerol 1,2-dinitrate
106. Monoacetin 1,3(or 2,3)dinitrate
107. 3-(2,4-dinitrophenoxy)-1,2-propanediol dinitrate
108. 1,3-Dipicrin 2-nitrate
109. 3-Chloro-1,2-propanediol dinitrate
110. 1-Monoglycolin trinitrate
111. 1-Monolactin trinitrate
112. 3-Methoxy-1,2-propanediol dinitrate
113. 1-Monopicrin dinitrate
114. Guanidine nitrate
115. Guanidine perchlorate
116. 1-Guanyl-3-nitrourea
117. N,N-Dichloroethylamine
118. 3,4,8,9,12,13-Hexoxa-1,6-diazabicyclo [4.4.4] tetradecane
119. 1,2,3,4,5,6-Benzenehexamethanol hexanitrate
120. Hexamethylenetetramine dinitrate
121. Hexamethylenetetramine diperchlorate
122. Hexamethylenetetramine monoperchlorate
123. 2,2',4,4',6,6'-Hexanitroazobenzene
124. 2,2',4,4',6,6'-Hexanitrobiphenyl
125. 2,2',4,4',6,6'-Hexanitrodiphenylamine
126. 2,2',3,4',6,6'-Hexanitrodiphenylamine
127. N,N-Dipicrylethanolamine nitrate
128. 2,2',4,4',6,6'-Hexanitrodiphenyl ether
129. 2,3',4,4',6,6'-Hexanitrodiphenyl ether
130. N,N'-Dipicrylethylenedinitramine
131. 1,3-Dipicrylguanidine
132. N-Methyl-2,2',4,4',6,6'-hexanitrodiphenylamine
133. 2,2',4,4',6,6'-Hexanitrodiphenyl sulfide
134. 2,2',4,4',6,6'-Hexanitrodiphenyl sulfone
135. 1,3-Dipicrylurea
136. Hexanitroethane
137. 2,2',4,4',6,6'-Hexanitrohydrazobenzene
138. 2,2',4,4',6,6'-Hexanitrooxanilide
139. Hexanitrosobenzene
140. Hydrazine monochlorate
141. N,N'-Bi(azidoformamide)
142. Hydrazine dinitrate
143. Hydrazine monoperchlorate
144. Hydrogen cyanide
145. Inositol hexanitrate
146. Inulin trinitrate
147. Iodoso and iodoxy compounds
148. Lactose octanitrate
149. Lead azide
150. Styphnic acid, lead salt
151. Maltose octanitrate
152. Mannitol hexanitrate
153. Melamine dinitrate
154. Mercuric fulminate
155. Methazonic acid
156. Methylamine nitrate
157. Nitroform, methylamine salt

TABLE 139 (cont'd)

C-

158. Methylamine monoperchlorate
159. 4-Methyl-2,6-dinitro-2,4,6-triazaheptane
160. N,N'-methylenebis(N-Nitrosohydroxylamine)
161. (Methylenedioxy)dimethanol dinitrate
162. Methanediol dinitrate
163. N-Methylethylenedinitramine
164. α-Methylglucoside tetranitrate
165. 1,2,3-Butanetriol trinitrate
166. Methylnitramine
167. Methyl nitrate
168. 2-Methyl-2-nitro-1,3-propanediol dinitrate
169. 2,2,4-Tris(hydroxymethyl)-4-methyl-1,3,5-pentanetriol hexanitrate
170. N-Ethylmethylenedinitramine
171. 5-Nitramino-1,2,4,1H-triazole
172. Pentaerythritol diglycolate tetranitrate
173. Nitroacetonitrile
174. p-Nitrobenzyl nitrate
175. α,2,4-Trinitrobenzeneazomethane
176. 5-Nitro-p-toluenediazonium 2-sulfonate
177. 5,5-Dimethyl-1-nitrohydantoin
178. 2-Nitroethanol
179. Nitroethylene polymer
180. 2-Nitroethanol nitrate
181. Nitroglycerin
182. Nitroguanidine
183. Nitroguanidine nitrate
184. 1-Nitrohydantoin
185. Nitromethane
186. 5-Methyl-1-nitrohydantoin
187. N-Methyl-N-nitroglycolamide nitrate
188. 2-Methyl-2-nitro-1-propanol nitrate
189. 2-Nitro-2-(m-nitrophenyl)-1,3-propanediol dinitrate
190. 1-Nitro-3-(nitrosoamino)guanidine
191. 3-Nitro-2-oxazolidone
192. α,α,m-Trinitrotoluene
193. 1-(p-Nitrophenyl)-1,2-ethanediol dinitrate
194. 2-Nitro-1-(o-nitrophenyl)ethanol nitrate
195. Dimethylnitrosamine
196. 2,3,5,6-Tetranitroso-1-4-dinitrobenzene
197. Nitrosoguanidine
198. Urea picrate
199. 5-Nitro-1H-tetrazole
200. Nitrourea
201. Nitrourea picrate
202. N-Methylethanolnitramine nitrate
203. Dipicryl lead
204. Cyclohexene ozonide
205. 2,2-Bis(methoxymethyl)-1,3-propanediol dinitrate
206. 2-(Hydroxymethyl)-2-(methoxymethyl)-1,3-propanediol trinitrate
207. Pentaerythritol tetranitrate
208. 2,3,4,5,6-pentanitroaniline
209. 1-(2,4-Dinitrophenyl)-2-(2,4,5-trinitrophenyl)ethanol
210. 2,2',4,4',6-Pentanitrodiphenyl ether

TABLE 139 (cont'd)

C-

211. 2,2',4,4',6-Pentanitrodiphenyl sulfone
212. Ethyl perchlorate
213. Acetyl peroxide
214. m-Phenylenediamine diperchlorate
215. α-Azidoformamidine picrate
216. Picric acid
217. Picryl chloride
218. Picryl fluoride
219. 1,2-Propanediol dinitrate
220. Propyl nitrate
221. Pyridine perchlorate
222. Quebrachitol pentanitrate
223. Sucrose octanitrate
224. Tetraazidoquinone
225. 4-Guanyl-1-(nitrosoaminoguanyl)-1-tetrazene
226. Tetramethylammonium perchlorate
227. 1,3,8,10-Tetraaza-5,6,12,13-tetroxacyclotetradecane-2,9-dione
228. 2-Hydroxy-1,1,3,3-cyclohexanetetramethanol pentanitrate
229. 2,2,6,6-Tetrakis(hydroxymethyl)cyclohexanone tetranitrate
230. 2-Hydroxy-1,1,3,3-cyclopentanetetramethanol pentanitrate
231. 2,2,5,5-Tetrakis(hydroxymethyl)cyclopentanone tetranitrate
232. 2,2-Bis(nitraminomethyl)-1,3-propanedinitramine
233. 2,3,4,6-Tetranitroaniline
234. 2,3,5,6-Tetranitroanisole
235. 3,3',5,5'-Tetranitro-p,p'-azoxytoluene
236. 1,2,3,5-Tetranitrobenzene
237. 3,3'-Oxydi-1,2-propanediol tetranitrate
238. 2,2',4,4'-Tetranitrodiphenyl ether
239. 1,1,2,2-Tetranitroethane
240. Tetranitromethane
241. 1,3,6,8-Tetranitronaphthalene
242. 2,3,4,6-Tetranitrophenol
243. N-Methyl-N,2,3,4,6-pentanitroaniline
244. N,2,3,4,6-pentanitroaniline
245. 3-Nitro-1,2,4,5-tetranitrosobenzene
246. 4,4'-Bis(N,N-dimethyl-2,6-dinitroaniline)
247. 2,3,4,6-Tetranitrotoluene
248. Tetrakis(2-hydroxyethyl)ammonium pentanitrate
249. N,N'-Dipicryl-2,2-bis(N,2,4,6-tetranitroanilinomethyl)-1,3-propanedinitramine
250. 1-(Aminoguanyl)-4-guanyl-1-tetrazene
251. 1H-Tetrazole
252. 5-Azido-1H-tetrazole
253. Tetryl
254. Triazenes
255. 1,2,4,1H-Triazole
256. 3,3,6,6,9,9-Hexamethyl-1,2,4,5,7,8-hexoxacyclononane
257. Hexahydro-1,3,5-trihydroxy-s-triazine trinitrate
258. 1,2-Propanedinitramine
259. 1,3-Propanediol dinitrate
260. 1,3-Propanediol diperchlorate
261. 2-Butyl-2-(hydroxymethyl)-1,3-propanediol trinitrate
262. 2-(Chloromethyl)-2-(hydroxymethyl)-1,3-propanediol trinitrate
263. 2-(Hydroxymethyl)-2-methyl-1,3-propanediol trinitrate
264. 2-(Hydroxymethyl)-2-nitro-1,3-propanediol trinitrate

TABLE 139 (cont'd)

C-

265. 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol trinitrate
266. Trinitroacetonitrile
267. 2,4,6-Trinitro-m-anisidine
268. 2,4,6-Trinitro-m-phenetidine
269. 3-Amino-2,4,6-trinitrophenol
270. Picramide
271. 2,4,6-Trinitroanisole
272. 2,4,6-Trinitrobenzaldehyde
273. 1,2,4-Trinitrobenzene
274. 1,3,5-Trinitrobenzene
275. 2,4,6-Trinitrobenzoic acid
276. 2,4,6-Trinitrobenzyl nitrate
277. 2,4,6-Trinitro-m-cresol
278. N,N-Dimethylpicramide
279. N,N'-Dimethyl-N,N',2,4,6-pentanitro-m-phenylenediamine
280. ?,?,?-Trinitro-7,8-dinitroso-2-naphthol
281. 2,2'-(2,4,6-Trinitro-m-phenylene)diethanol dinitrate
282. 3-Ethyl-2,2,3-trinitropentane
283. N^2,N^4,N^6-Trinitromelamine
284. 2,4,6-Trinitromesitylene
285. 2-Methyl-2,3,3-trinitrobutane
286. N^1-Methyl-N^1,2,4,6-tetranitro-m-phenylenediamine
287. N-Methyl-N,2,4,6-tetranitro-m-anisidine
288. N-Methyl-N,2,4,6-tetranitro-m-phenetidine
289. 3-(Methylnitramino)-2,4,6-trinitrophenol
290. N-Methyl-N,2,4,6-tetranitro-m-toluidine
291. 3-Methyl-2,2,3-trinitropentane
292. N-Methylpicramide
293. 1,3,8-Trinitronaphthalene
294. 2,4,6-Trinitrophenetole
295. 2-(2,4,6-Trinitrophenoxy)ethanol nitrate
296. Picryl azide
297. N-Butyl-N,2,4,6-Tetranitroaniline
298. 3-(N,2,4,6-Tetranitroanilino)-1,2-propanediol dinitrate
299. 2,4,6-Trinitro-m-phenylenediamine
300. N-Ethyl-N,2,4,6-tetranitroaniline
301. 2-Picrylethanol nitrate
302. Picrylguanidine
303. Picrylhydrazine
304. N-Methoxy-N,2,4,6-tetranitroaniline
305. 2-(N,2,4,6-Tetranitroanilino)-1-butanol nitrate
306. N,2,4,6-Tetranitroaniline
307. 2-(N,2,4,6-Tetranitroanilino)ethanol nitrate
308. 2-(Hydroxymethyl)-2-(N,2,4,6-tetranitroanilino)-1,3-propanediol trinitrate
309. Trinitrophloroglucinol
310. Styphnic acid
311. 2,2'-(2,4,6-Trinitro-m-phenylenedioxy)diethanol dinitrate
312. 2,4,6-Trinitrostilbene
313. 2,4,6-Trinitrotoluene
314. 2,3,4-Trinitrotoluene
315. 1,3,5-Triazido-2,4,6-trinitrobenzene
316. N,N',N"-Trimethyl-N,N',N",2,4,6-hexanitro-1,3,5-benzenetriamine
317. Triethanolamine tetranitrate

TABLE 139 (cont'd)

C-

318. 2,4,6-Trinitro-m-xylene
319. 1,1',1"-Tris(methylnitramino)trimethylamine
320. Urea nitrate
321. 4-Halo-1-buten-3-yne polymer
322. Vinyl nitrate polymer
323. α,α'-Diazido-p-xylene
324. n-Propyl picrate
325. Allyl picrate
326. 2-Propynyl picrate
327. Nitroform
328. Methylenedinitramine
329. N-Methyl-N,2,3,4,5-pentanitroaniline
330. 2,2,2-Trinitroethanol
331. 1,3-Bis(2,2,2-trinitroethyl)urea
332. Ethylenediamine dinitroform salt
333. N,N'-Dichloroethylenedinitramine
334. (2,4-Dinitrophenyl)hydrazine
335. 1,1-Dinitro-N-(1-nitroethylidene)ethylamine oxide
336. α,α,α-Trifluoro-3,5-dinitrotoluene
337. Bis(2,2,2-trinitroethyl)nitramine
338. 5-Amino-1H-tetrazole hydrate
339. 5-Amino-1H-tetrazole nitrate
340. 2,2,2-Trinitroethanol 4,4,4-trinitrobutyrate
341. Tris(2,2,2-trinitroethyl)phosphate
342. 5-Amino-1H-tetrazole
343. 2,2,3,3-Tetranitrobutane
344. N,N'-Methylenebis(N-nitroformamide)
345. 5-(2,2,2-Trinitroethylamino)-1H-tetrazole
346. Methylenedinitramine dihydrazine salt
347. 2,4,6-Trinitro-2,4,6-triazaheptane-1,7-diol dinitrate
348. ω-Azido-N-nitroformamidine
349. 4,6-Dinitramino-s-triazin-2-ol
350. N,N'-Methylenebis(2,2,2-trinitroacetamide)
351. 2,2-Dinitroacetamide
352. Hydrazine mononitrate
353. Hydrazine
354. 5,5'-Hydrazodi-1H-tetrazole
355. By-product from Hedina synthesis
356. 2,4-Dinitrothiophene
357. 4-Methyl-3,5-dinitro-1,2,4,4H-triazole
358. Methylenebis(nitroimino)dimethanol dinitrate
359. 5-Nitramino-1H-tetrazole
360. Azidodithioformic acid
361. Azidosulfonic acid
362. Aniline
363. p-Azidoaniline perchlorate
364. 2-Azido-4,6-dinitrophenol
365. Carbonyl azide
366. p-Diazidobenzene
367. 1,2-Diazidoethane
368. 1,3-Diazidopropane
369. α,α'-Diazido-2,5-dinitro-p-xylene
370. 1,3,5-Triazido-2,4-dinitrobenzene

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TABLE 139 (cont'd)

C.

371. Hydrazinium azide
372. ω-Azido-p-nitrotoluene
373. 2,4-Diazido-1,3,5-trinitrobenzene
374. 1,2,3-Benzoxadiazole
375. 5,7-Dinitro-1,2,3-benzoxadiazole-4,6-diol
376. 5,7-Dinitro-1,2,3-benzoxadiazol-4-ol
377. 5,7-Dimethyl-4,6-dinitro-1,2,3-benzoxadiazole
378. 5-Hydroxy-6-nitro-1,2,3-benzoxadiazole-4,7-dione
379. 4,5,6,7-Tetranitro-1,2,3-benzoxadiazole
380. Benzenediazonium nitrate
381. p-(2,4-Dinitroanilino)benzenediazonium nitrate
382. 1,5-Dichloro-2,4-dinitrobenzene
383. 3,5-Dinitroanisole
384. 1,2-Dinitroethane
385. 2,5-Dinitrophenol
386. 2,6-Dinitrophenol
387. 2,2-Dinitropropane
388. 1,3-Dinitropropane
389. 4,6-Dinitroresorcinol
390. 2,6-Dinitrotoluene
391. 3,5-Dinitro-o-xylene
392. Glycerol 1,3-dinitrate
393. (Nitromethoxy)methanol nitrate
394. 1,2-Ethanediol polymer dinitrate
395. 1,2,4-Butanetriol trinitrate
396. 2,3',4,4',6-Pentanitrodiphenyl ether
397. Ammonium perchlorate
398. Ethylenediamine diperchlorate
399. 1,2-Propanediamine diperchlorate
400. 1,3-Propanediamine diperchlorate
401. Bis(2,2,2-trinitroethyl)amine
402. ω-Azidoformamidine perchlorate
403. 2-Methyl-1,3-butanediamine diperchlorate
404. 1-Naphthylamine perchlorate
405. 3-(Perchloratomercuri)-1,2,4-oxadimercuretan-3-al
406. Benzoyl peroxide
407. Di-2,4-cyclopentadien-1-yl peroxide
408. Picryl hydroperoxide, sodium salt
409. 2,3,4,6-Tetranitroanisole
410. 2,3,5-Trinitrotoluene
411. 2,3,6-Trinitrotoluene
412. 2,4,5-Trinitrotoluene
413. 3,4,5-Trinitrotoluene
414. 3,4,5-Trinitro-o-xylene
415. 3,4,6-Trinitro-o-xylene
416. 2,3,5-Trinitro-p-xylene
417. (Nitroimino)diacetonitrile
418. Dimethylnitramine
419. 1,7-Dinitro-1,4,7-triazaheptane
420. 1,10-Dinitro-1,4,7,10-tetrazadecane
421. 1-Methyl-3-nitroguanidine
422. Nitramide
423. N-Methyl-N,2,4,5,6-pentanitro-m-toluidine

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TABLE 139 (cont'd)

C-

424. 2-tert-Butoxyethanol nitrate
425. Tetrahydrofuran-3,4-diol dinitrate
426. 1,3-Diethoxy-2-propanol nitrate
427. 2-Propanol nitrate
428. Mannitan tetranitrate
429. Pentaerythritol diacetate dinitrate
430. Pentaerythritol diformate dinitrate
431. Pentaerythritol lactate tetranitrate
432. Pentaerythritol m-nitrobenzoate trinitrate
433. Sorbitol hexanitrate
434. 2,2,2-Trinitroethanol nitrate
435. Aminoguanidine nitrate
436. Guanylurea nitrate
437. Hydroxylamine nitrate
438. N-Methylhydroxylamine nitrate
439. Piperazine dinitrate
440. Succinonitrile
441. Malononitrile
442. 1,4-Dibromo-2,3-dinitrobenzene
443. 1-Bromo-2,4-dinitrobenzene
444. 2,4-Dinitromesitylene
445. 3,5-Dinitrosalicyclic acid
446. 1,3,5-Tribromo-2,4-dinitrobenzene
447. 2,2',4,4',6,6'-Hexanitrooxybenzene
448. 2,2',4,4',6,6'-Hexanitrobibenzyl
449. 3,3'-Azobis(2,4,6-trinitrophenol)
450. 1,3-Dimethyl-1,3-dipicrylurea
451. 2,2',4,4',6,6'-Hexanitrostilbene
452. 2,2',4,4',6,6'-Hexanitro-3,3',5,5'-biphenyltetrol
453. 2,2',4,4'-Tetranitrobenzophenone
454. Tetranitroresorcinol
455. 2,4,5,6-Tetranitro-m-xylene
456. 1,3,5-Trichloro-2,4,6-trinitrobenzene
457. Benzene
458. 2-Ethyl-1,3,5-trinitrobenzene
459. 1-Methyl-1,3-dinitrosoguanidine
460. Benzene triozonide
461. Biphenyl tetraozonide
462. Naphthalene diozonide
463. N,N,N',N'-Tetrabromoethylenediamine
464. N,N'-Ethylenebis(N-chloro-p-nitrobenzamide)
465. 1,4-Dibromopiperazine
466. N,N-Dichloroformamide
467. 2,3-Butanediol dinitrate
468. 3-(Chloratomercuri)-1,2,4-oxadimercuretan-3-al
469. (Chloratomercuri)mercuricacetaldehyde
470. Methylenebis(N-nitrosohydroxylamine) anhydrous sodium salt
471. Methylenebis(N-nitrosohydroxylamine) monohydrate sodium salt
472. Methylenebis(N-nitrosohydroxylamine) diammonium salt
473. Methylenebis(N-nitrosohydroxylamine) monoammonium salt
474. Methylenebis(N-nitrosohydroxylamine) anhydrous cadmium salt
475. Methylenebis(N-nitrosohydroxylamine) dihydrate cadmium salt
476. Methylenebis(N-nitrosohydroxylamine) lead salt
477. Methylenebis(N-nitrosohydroxylamine) bis(diethanolamine dinitrate) salt

TABLE 139 (cont'd)

C-

478. Methylenebis(N-nitrosohydroxylamine) monohydroxylamine salt
479. Dipicryl mercury
480. 1-Nitronaphthalene
481. 1,5-Dinitronaphthalene
482. 1,8-Dinitronaphthalene
483. 1,3,5-Trinitronaphthalene
484. 1,4,5-Trinitronaphthalene
485. 2-Methyl-1,2,3-propanetriol trinitrate
486. 1,4,5,8-Tetranitronaphthalene
487. 1,3,5,8-Tetranitronaphthalene
488. 5-[Bis(2,2,2-trinitroethyl)amino]-1H-tetrazole
489. 3-(2-Hydroxyethoxy)-1,2-propanediol trinitrate
490. 1-Hydroxy-5,5'-azodi-1H-tetrazole
491. 5,5'-Azodi-1H-tetrazole
492. 5,5'-Bis(1-hydroxy-1H-tetrazole)
493. 5,5'-Bi-1H-tetrazole
494. Triazeto[4,1-e]tetrazole
495. 3,4-Benzylidene-4-guanyl-1-(1H-tetrazol-5-yl)-1-tetrazene
496. 3-Phenyl-1-(1H-tetrazol-5-yl)-1-tetrazene
497. 4-Guanyl-1-(1H-tetrazol-5-yl)-1-tetrazene
498. 1-Hydroxy-1H-tetrazole-5-methanol
499. 1-Hydroxy-5-nitro-1H-tetrazole
500. 1-Hydroxy-1H-tetrazole-5-methanol nitrate
501. 1-Hydroxy-1H-tetrazole
502. 5-(2,4,6-trinitroanilino)-1H-tetrazole
503. 1(or5)-Amino-5(or 1)-nitramino-1,2,4,1H-triazole
504. 5-(Nitrosoamino)-1,2,4,1H-triazole-3-carboxylic acid
505. Biacetylenedicarboxylic acid
506. 2,6-Dinitro-p-cresol
507. m-Nitroaniline
508. Phenol
509. p-Nitrophenol
510. Pentanitrophenol
511. Phenylhydrazine
512. (p-Nitrophenyl)hydrazine
513. (2,3,4,6-Tetranitrophenyl)hydrazine
514. (2,3,4,5,6-Pentanitrophenyl)hydrazine
515. Nitrobenzene
516. Pentanitrobenzene
517. Hexanitrobenzene
518. 1,1,2,2-Ethanetetranitramine
519. 2-Nitrothiophene
520. 3-Methyl-2-nitrosothiophene
521. 3-Methyl 2,4-dinitrothiophene
522. Dinitroacetylene
523. 1,1,1,3,5,5,5-Heptanitropentane
524. 3,4,5-Triamino-1,2,4,4H-triazole
525. Guanazole
526. 4-Amino-1,2,4,4H-triazole-3,5-diol
527. Urazole
528. 1,2,3-Triaminoguanidine
529. 1,2,3-Triaminoguanidine dinitrate
530. 1,3-Diaminoguanidine
531. 1,3-Diaminoguanidine nitrate

TABLE 139 (cont'd)

C-

532. Oxalic acid, monohydrazine salt
533. Oxalic acid, bis(hydroxylamine)salt
534. Oxalic acid, semicarbazide salt
535. Oxalic acid, aminoguanidine salt
536. Carbohydrazide
537. Oxalic acid, monocarbohydrazide salt
538. 1-Carbamylcarbohydrazide
539. 1,5-Dicarbamylcarbohydrazide
540. 2,4-Diamino-s-triazine
541. N,N'-Bi(ethyl carbamate)
542. Biurea
543. N-Guanidinooxamic acid
544. 5-Amino-1,2,4,1H-triazole-3-carboxylic acid
545. 1,2,3-Triaminoguanidine monohydrochloride
546. 2,4-Diamino-6-methyl-s-triazine dinitrate
547. Tetrahydro-1,3,5,7-tetraimino-s-triazolo[a]-s-triazole
548. 2,4-Diguanidino-s-triazine dinitrate
549. Cyanuric trihydrazide
550. 1-Cyanoguanidine
551. Melamine
552. Oxalic dihydrazide
553. Oxamide
554. Cyanuric acid
555. 6-Nitramino-s-triazine-2,4-diol
556. m-Nitrotoluene
557. o-Nitrophenol
558. m-Nitrophenol
559. m-Nitrophenetole
560. o-Nitrophenetole
561. p-Nitrophenetole
562. o-Nitroaniline
563. p-Nitroaniline
564. o-Nitroacetanilide
565. m-Nitroacetanilide
566. p-Nitroacetanilide
567. 1,1,1-Trinitroethane
568. 2,4-Dinitrophenetole
569. 1,1,2-Trinitroethane
570. 2-Methyl-2,3,3-trinitropentane
571. Picramic acid
572. p-Nitrobenzaldehyde
573. 1,2,6-Hexanetriol trinitrate
574. 2,2-Dinitro-1,3-propanediol
575. 4,4-Dinitropimelic acid
576. 1,1,1,3-Tetranitropropane
577. 5,5,5-Trinitro-2-pentanone
578. Methyl 4,4,4-trinitrobutyrate
579. 1,1,1-Trinitro-2-propanol acetate
580. 4,4,4-Trinitro-N-(2,2,2-trinitroethyl)butyramide
581. 1,3-Bis(2,2,2-trinitroethyl)-2-imidazolidone
582. 4,4-Dimethyl-5,5,5-trinitro-2-pentanone
583. Diethyl (2,2,2-trinitroethyl)malonate
584. N,N'-Bis(2,2,2-trinitroethyl)-1,4-piperazinedicarboxamide
585. Urea

TABLE 139 (cont'd)

C-

586. Guanidinoacetic acid
587. Ethylurea
588. 1,3-Bis(hydroxymethyl)urea
589. 2-Imidazolidone
590. 1-Methyl-1-phenylhydrazine
591. Hydrazobenzene
592. Tetraphenylhydrazine
593. Ethylnitramine
594. 1,3-Dinitroimidazolidine
595. Acetone
596. 3,3'-(Nitroimino)dipropionitrile
597. 4,4-Dimethyl-5-nitro-2-pentanone
598. 1-Picrylaziridine
599. 2-(2-Nitrovinyl)furan
600. 2-Nitro-5-(2-nitrovinyl)furan
601. 2-(2,4-Dinitrophenyl)-5-nitro-2H-benzotriazole
602. α,α-Dinitrotoluene
603. N-(2,4-Dinitrophenyl)diethanolamine
604. 2-(2,4-Dinitroanilino)-2-(hydroxymethyl)-1,3-propanediol
605. 2-(2,4-Dinitroanilino)-1,3-propanediol
606. 2-[2-(2,4-Dinitroanilino)ethylamino]ethanol
607. Ethylenebis(ethyl nitrocarbamate)
608. 1,1'-Ethylenebis(3-nitrourea)
609. 1-(o-Nitrophenyl)-1,2-ethanediol dinitrate
610. 1,2-Propanediol 2-nitrate 1-(5-nitro-2-furoate)
611. N-Picryldiethanolamine dinitrate
612. N-Methyl-N,5-dinitro-2-furamide
613. N,N'-Dimethyloxamide
614. N-Methylglycolamide
615. 5,5-Dimethylhydantoin
616. 3,6-Dimethyl-2,5-piperazinedione
617. Nitroethane
618. 1-Nitropropane
619. 2-Nitropropane
620. 1-Nitrobutane
621. 2-Nitrobutane
622. 1,1'-(2-Hydroxytrimethylene)bis(3-nitroguanidine) mononitrate
623. 3-[2,2,2-Tris(hydroxymethyl)ethoxy]-1,2-propanediol pentanitrate
624. 2-(Allyloxymethyl)-2-(hydroxymethyl)-1,3-propanediol trinitrate
625. 1-Nitro-3-(1-hydroxyethyl)guanidine nitrate
626. 2-(Hydroxymethyl)-2-(propoxymethyl)-1,3-propanediol trinitrate
627. 2,2-Bis(allyloxymethyl)-1,3-propanediol dinitrate
628. 1-Nitro-3-(2,2,2-trinitroethyl)guanidine
629. Ethyl 4,4,4-trinitrobutyrate
630. 1-Nitro-3-(2,3-dihydroxypropyl)guanidine dinitrate
631. 1-Nitro-3-(2-hydroxyethyl)guanidine nitrate
632. 1,5-Pentanediol dinitrate
633. 2,3,3,4,5-Pentamethyl-1,1,1,5-tetranitrohexane
634. 1,6-Hexanediol dinitrate
635. 1,4-Butanediol dinitrate
636. Bis(3,3,3-trinitropropyl) sulfone
637. Oxalimidic dihydrazide dinitrate
638. Diethyl 3,3,3-trinitro-1-propanephosphonate
639. 4,4,4-Trinitrobutyramide

TABLE 139 (cont'd)

C-

640. Dinitroform, dioxane addition compound
641. 5,5,5-Trinitro-2-pentanone N-nitroguanylhydrazone
642. 5,5,5-Trinitro-2-pentanone semicarbazone
643. 2,2-Dinitro-1-propanol acrylate
644. Methyl nitroacetate
645. 2,5-Hexanediol dinitrate
646. n-Butyl 4,4,4-trinitrobutyrate
647. Diethyl 3-hydroxyglutarate nitrate
648. 1,2,5-Pentanetriol trinitrate
649. 1,2-Butanediol dinitrate
650. 1,5-Dinitro-2,3-dinitrosobenzene, potassium salt
651. 1,4-Dinitro-2,3-butanediol dinitrate
652. 3,3-Dinitro-1,5-pentane diisocyanate
653. 2,2,4,4-Tetranitro-1-butanol acetate
654. 3,3-Dinitro-1,5-pentanediamine
655. Methyl 4,4,6,6-tetranitrocaproate
656. 2,2,2-Trinitroethanol methacrylate
657. 2,2,4,4-Tetranitro-1,5-pentanediol
658. 2-Nitramino-2-imidazoline
659. 2-Nitramino-1-nitro-2-imidazoline
660. 1,4,5,6-Tetrahydro-2-nitraminopyrimidine
661. N-Nitroethyleneimine polymer-diol dinitrate
662. 2,16-Dimethyl-3,6,9,12,15-pentanitro-3,6,9,12,15-pentazaheptadecane-2,16-dicarbonitrile
663. 2,13-Dimethyl-3,6,9,12-tetranitro-3,6,9,12-tetrazatetradecane-2,13-dicarbonitrile
664. 2,10-Dimethyl-3,6,9-trinitro-3,6,9-triazaundecane-2,10-dicarbonitrile
665. 2,7-Dimethyl-3,6-dinitro-3,6-diazaoctane-2,7-dicarbonitrile
666. 2-Nitropropene polymer
667. 1-Ethyl-3-nitroguanidine
668. 1-Nitro-3-propylguanidine
669. 1-Butyl-3-nitroguanidine
670. 1-Amyl-3-nitroguanidine
671. Guanidine
672. Pyridine
673. Ethyl acetate
674. 4,4'-Isopropylidenebis(6-nitro-o-cresol)
675. N-Ethyl-N-nitrosoaniline
676. N-Nitrosodiphenylamine
677. 1,5-Dimethyl-1H-tetrazole
678. 1-Phenyl-1H-tetrazole
679. 5-Phenyl-1H-tetrazole
680. 5-Methyl-1-phenyl-1H-tetrazole
681. 5-Methyl-2-phenyl-2H-tetrazole
682. 1,5-Diphenyl-1H-tetrazole
683. 2,5-Diphenyl-2H-tetrazole
684. 1-Phenyl-1H-tetrazol-5-ol
685. 2-Phenyl-2H-tetrazole-5-carboxylic acid
686. Ethyl N-1H-tetrazol-5-ylcarbamate
687. N-1H-tetrazol-5-ylacetamide
688. 1H-Tetrazol-5-ylguanidine
689. 5-Nitramino-1H-tetrazole monoguanidine salt
690. Benzldehyde, 1H-tetrazol-5-ylhydrazone

TABLE 139 (cont'd)

C-

691. Hydrazine hydrate
692. 4,4'-Cyclohexylidenebis(2,6-dinitrophenol)
693. 2,2'-Hydrazodiisobutyronitrile
694. Acetic 1,2-diphenylhydrazide
695. N,N'-Biacetanilide
696. N,N'-Bibenzamide
697. Malonic dihydrazide
698. Succinic dihydrazide
699. Thiophane
700. Catechol

SECTION XVII
Calculation of Power (nRT) of Explosives Compounds and Mixtures

A. Abstract

A previously developed method for the calculation of the impulse propellants has been successfully adapted to the calculation of powers high explosives, relative to TNT. The success of this method is indicated by the correlation achieved between the calculated power (nRT) and the measured ballistic mortar values for 111 pure compounds, 56 mixtures of organic explosives and 30 mixtures of explosives containing metals. In the case of the pure compounds, the average deviation is +1.6 while the standard deviation is 6.7. In the case of the mixture calculations, the average deviation is +0.1 while the standard deviation is 5.8. Corresponding figures for the metallized mixtures are -0.8 for average and 7.8 for standard deviations.

By using the system described in Section XVI for calculating the heat of combustion, and the method described here for calculating nRT, it is possible to evaluate a pure compound or mixture, as to power, by a few simple calculations without the necessity for making and testing the compound.

B. Introduction

This section describes a simplified method for calculating the power of a high explosive (pure compound or mixture) from thermodynamic data which gives results bearing a direct, virtually equivalent, relation to the power of the explosive as measured in the ballistic mortar and the new-type spherical lead block. Power as used here and as measured in the ballistic mortar is that force exercised by an explosive burning in an enclosed space, large enough only to contain the explosive. Thus, it is energy developed at virtually constant volume. All thermodynamic data are therefore referred to constant volume.

Calculation of the PV work product (F = nRT) according to the simplified procedure of Hirschfelder has been used for propellant powders for some time (10). The application of this same method to explosives has been described briefly (6). This presentation extends the calculations and data presented previously. Calculations of a large number of pure compounds, mixtures of organic compounds and metallic mixtures indicate the value of this method as a tool for quickly evaluating the power of an explosive.

In this method, one hundred times the quotient of the calculated energy divided by the energy of an equal weight of TNT expresses the power of the explosive in terms of per cent TNT.

Previous simplified methods employed in the calculation of power of high explosives have assumed an overall specific heat for the product gases formed in the detonation (1). The system described in this report, by applying the Hirschfelder method of calculating temperature, takes into account the variation in specific heat for the various product gases formed over the particular temperature range involved. Thus it is believed that explosion-temperatures calculated in the method described in this report are somewhat more realistic, although it is not claimed that they are the true values, since they do not take into account the dissociation of the product gases. The reaction products which are taken into account are governed by the assumptions stated on page 580.

It is also possible to correlate the nRT values obtained with those measured in the new type spherical lead block, a test method which is to be described in a forthcoming report. This correlation is shown in Table 147 and briefly discussed.

One method for calculating power of high explosive used in the past was the so-called "characteristic product" (Berthelot) which gave power as per cent TNT by the formula

$$P\ (\%\ TNT) = 0.003594\ M \cdot H_E$$

in which M = moles of gas per kg. of explosive

H_E = heat of explosion in kcal/kg.

This system has been applied to a number of compounds and mixtures (4, 5). Comparison of results by the nRT and Berthelot methods of calculation shows distinct advantages of the former as given in the following:

nRT System	Berthelot System
1) Correlates observed ballistic mortar power values with calculated values, on a 45° line, thus giving identical figures. (See Figures 80, 81 and 82).	1) Correlates calculated values with observed lead block values on a straight line, not 45°. (Figure 64 Reference (5)); and with ballistic mortar on a curved line (Figure 57 Reference (5)).
2) Applicable to primary and secondary plosophores, auxoplosives, and mixtures including those containing metallic elements.	2) The same correlations do not apply to mixtures yielding products partly non-gaseous; i.e., metallized mixtures. (Figure 56 Reference (5)).

nRT System	Berthelot System
3) Includes calculation of a realistic value for explosion temperature, necessary when gas dissociation is considered.	3) No temperature calculated.
4) Results of power calculation are capable of being expressed in meaningful units, e.g., cal/g. ft. lbs./g, etc.	4) Results are comparative only.

A series of the Berthelot calculations have been made and compared with the observed Ballistic Mortar values (5). Although there was no direct, straight-line relationship shown, it was possible to formulate an idealized curve.

C. Discussion

The simplified system presented here is based upon the determination of the pV work product of the gases of detonation. The common expression for this work product is: pV = nRT, here written as

$$pV = R \cdot T \cdot \Sigma n \qquad (1)$$

where R is the universal gas constant (1.987 cal/°K/mole), T is the adiabatic flame temperature, °K, and Σn is the number of moles of gas formed from one mole of explosive. The parameter, Σn, is obtained by writing the detonation equation. The flame temperature, T, must be estimated from the equation

$$T = 298 + \frac{Q^v_E}{\Sigma nC_v} \times 10^3 \qquad (2)$$

where Q^v_E is the heat of explosion at constant volume in kcal/mole, n is the moles of each gas formed, and C_v is the average heat capacity in cal/mole of each gas, at constant volume, over the range 298 to T. This temperature, T, is actually obtained by a process of iteration, using the specific heat values tabulated. (Table 149). Examples of detailed calculations are given in Subsection D below.

The substitution of appropriate quantities for Σn and T in equation (1) gives a value, which when divided by a corresponding value for TNT, results in a power for the explosive, in terms of TNT, which compares directly with observed ballistic mortar and spherical lead block measurements.

It is fully recognised that in this very simple method of calculation there have been discounted several factors, among which are the possibility of dissociation of the product gases, the effect of γ (the ratios of

specific heats, C_p/C_v), and deviations from the perfect-gas law.

Dissociation of the product gases would result in an increase in Σn and a corresponding decrease in the adiabatic flame temperature, thus counterbalancing, at least to some extent, the effects described.

It can be shown that in a simplified system such as this, γ has little effect upon the final relative values. This is due to the fact that for all practical purposes only diatomic and triatomic gases are produced in the detonation. A review of some of the more typical high explosives reveals that γ varies over an extremely small range, (Table 140) thus making a refined treatment of this parameter unnecessary in a system where only relative values are involved.

Table 140
Ratio of Specific Heats, γ, for Product Gases for Selected High Explosives

COMPOUND No.	Name	γ for Product Gases, 298°K
22	HMX	1.37
23	RDX	1.37
35	Diethanolnitramine dinitrate	1.36
37	Diethylene glycol dinitrate	1.38
208	2,3,4,5,6-Pentanitroaniline	1.36
216	Picric acid	1.39
233	2,3,4,6-Tetranitroaniline	1.38
240	Tetranitromethane	1.39
313	2,4,6-Trinitrotoluene	1.40
328	Methylenedinitramine, MEDINA	1.35
331	1,3-Bis(2,2,2-trinitroethyl)urea	1.34
337	Bis(2,2,2-trinitroethyl)nitramine, HOX	1.37
343	2,2,3,3-Tetranitrobutane	1.36
	Average	1.37

Even at high temperatures, and thus lower γ's, the deviation from an average value is very small.

The heats of combustion used in these calculations were obtained by the method described in Section XVI. It was found that, generally, the use of calculated in place of observed heats of combustion gave nRT values which correlated better with the observed ballistic mortar values. The

specific heats, C_p/C_v), and deviations from the perfect-gas law.

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observed heats of combustion were used in the calculations shown in the original presentation of this method (6).

Other thermodynamic data used were derived from OSRD Report 547 (10), the Bureau of Standard Tables (7), and the open literature (2, 9, 11, 12). These data, as used in these calculations, are given in Table 141, 142 and 149.

Table 141 gives the energy values required for converting H_2O liquid to H_2O gas and heats of combustion to heats of explosion.

Table 141
Thermodynamic Data for Selected Reactions

	Constant * Pressure	Converted to Constant Volume
H_2O (liq.) $\longrightarrow$ H_2O (gas)	10.519	9.927 kcal/mol
$C + O_2 \longrightarrow CO_2$	94.052	93.460
$CO + 0.5\ O_2 \longrightarrow CO_2$	67.636	67.341
$H_2 + 0.5\ O_2 \longrightarrow H_2O$ (gas)	57.798	57.502

* Reference (7)

Table 142 gives the heats of combustion and heats of fusion and vaporization for the metals and their corresponding oxides entering into these calculations.

Table 142
Thermodynamic Data for Selected Metals and their Corresponding Oxides

	Q_C^V (H_2O gas)	Q_{fusion}	$Q_{vaporization}$	$Q_{sublimation}$	b.p., °K
Al	199.54 a/	2.6 a/	67.9 a/	70.5	2330*
Al_2O_3	--	2.6 a/	65.6 c/	91.6	2523 b/
B	151.0 a/			97.2 b/	2823 b/
B_2O_3	--	5.3 a/	77 a/	82.3	>1800 b/
Mg	143.0 a/	2.2 a/	31.5 a/	33.7	1393 a/
MgO	--	18.5 a/	100.7 c/	119.2	3823 a/

a/Bureau of Standards value (7); b/Handbook; c/ Estimated; *Vaporizes at 2073°K

In Table 149 are given the specific heats at constant volume, for 10°K intervals, for the assumed products of detonation. In extending these specific heat data to 7000°K it is fully realized that such extrapolation of data, infrequently measured for temperatures above 2000°K, is at best guess-work, but the lack of data, particularly for the metal oxides, forced such extrapolations. It should be noted that in spite of these considerable extrapolations, the degree of accuracy attained in the final values (% TNT) is good and appears to be in no way related to the temperature range involved, at least up to 5000°K.

Finally, in making these calculations, it was necessary to make certain assumptions as to the products of detonation. These assumptions are:

1. The oxygen present is used first to burn the carbon to CO, then the hydrogen to H_2O, and finally the CO to CO_2. This follows the Kistiakowsky-Wilson assumption.

2. If a metal is present, it is oxidized fully before any CO is formed.

3. Any free carbon remaining unburned is considered a solid and is, therefore, not added into the number of moles of gas formed.

4. The metal oxides assumed to be formed remain solids unless the calculated adiabatic flame temperature exceeds the boiling point of the oxide. If the boiling point is exceeded,, the heat necessary to vaporize the quantity of oxide is subtracted from the heat of explosion and the adiabatic flame temperature is recalculated. This may result in a calculated temperature less than the boiling point, indicating that only part of the oxide is vaporized.

The accuracy of this method of calculation of power is illustrated in Figures 80, 81 and 82 which show the direct relationship between calculated power and observed ballistic mortar values for 111 pure compounds, 56 organic mixtures and 30 metallized mixtures. Applying simple statistical methods to these data, it may be shown that the average deviation of the observed from the calculated is +1.6 for the pure compounds (eliminating 6 as discussed below), +0.1 for the organic mixtures and -0.8 for the metallized mixtures. The standard (root-mean square) deviations, from the mean, are 6.7 for the pure compounds, 5.8 for the organic mixtures and 7.8 for the metallized mixtures.

Figure 83, drawn to show the statistical scatterings for the pure compounds, mixtures and metallized mixtures, indicate that these scatterings are generally normal. This leads to the conclusion that the deviations are due largely to personal errors and are therefore not inherent in the system or in the compounds.

The summarized results of the calculations are given in Tables 143, 144 and 145. Ballistic mortar data were taken from Parts I and III of this series (3, 5).

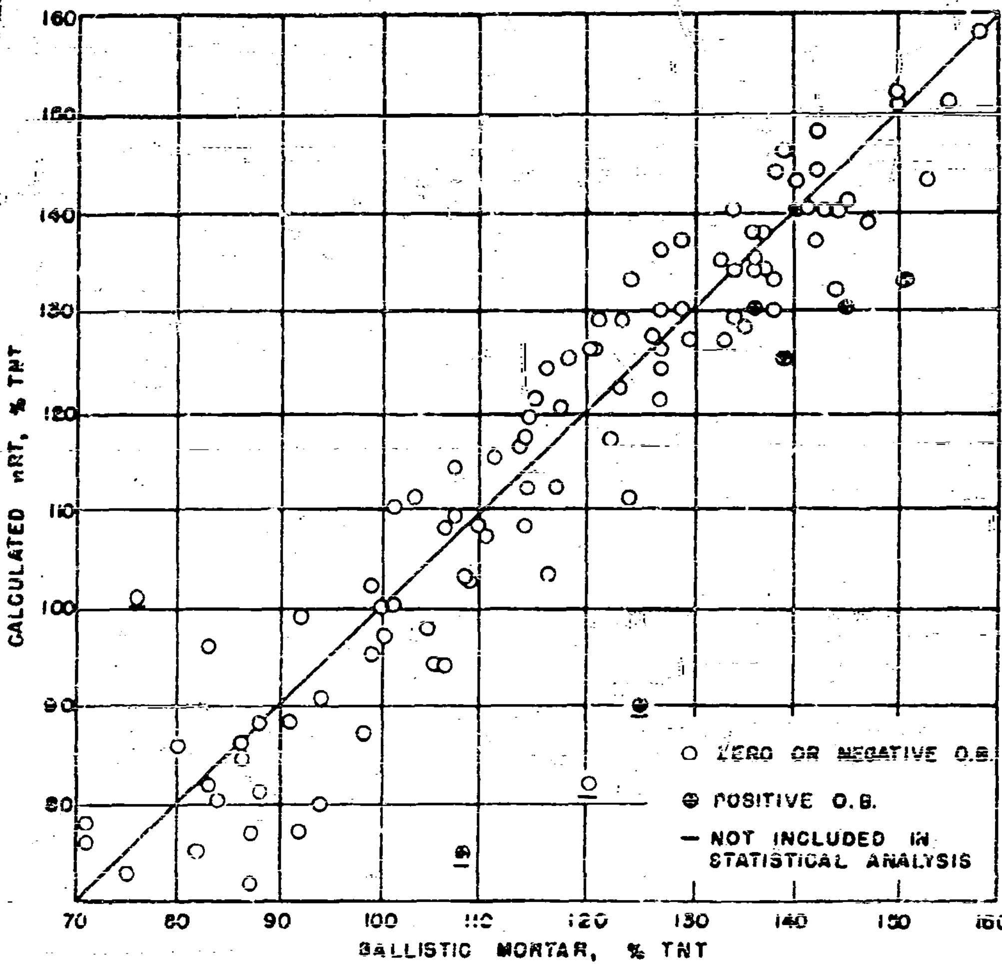

FIGURE 80

COMPARISON OF BALLISTIC MORTAR AND CALCULATED nRT FOR PURE EXPLOSIVE COMPOUNDS

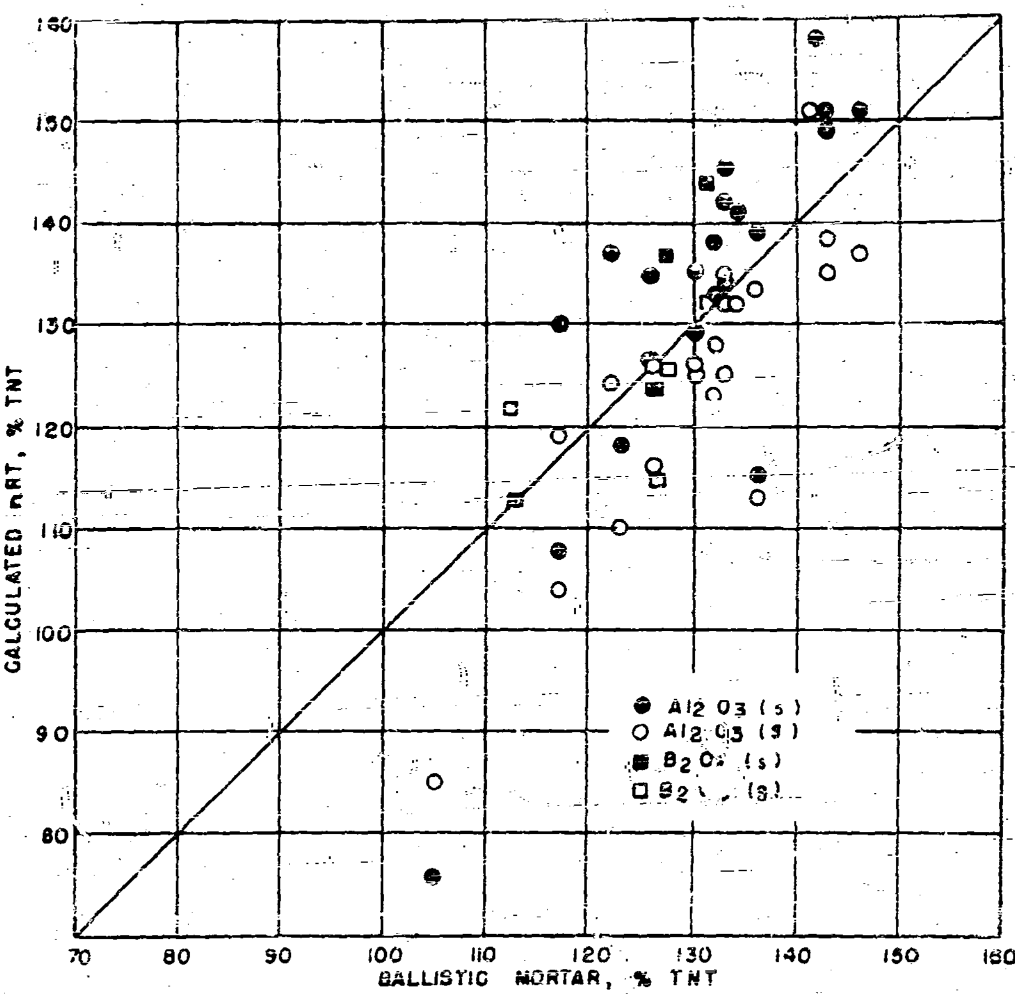

FIGURE 82
COMPARISON OF BALLISTIC MORTAR AND CALCULATED nRT FOR EXPLOSIVE METALLIC MIXTURES

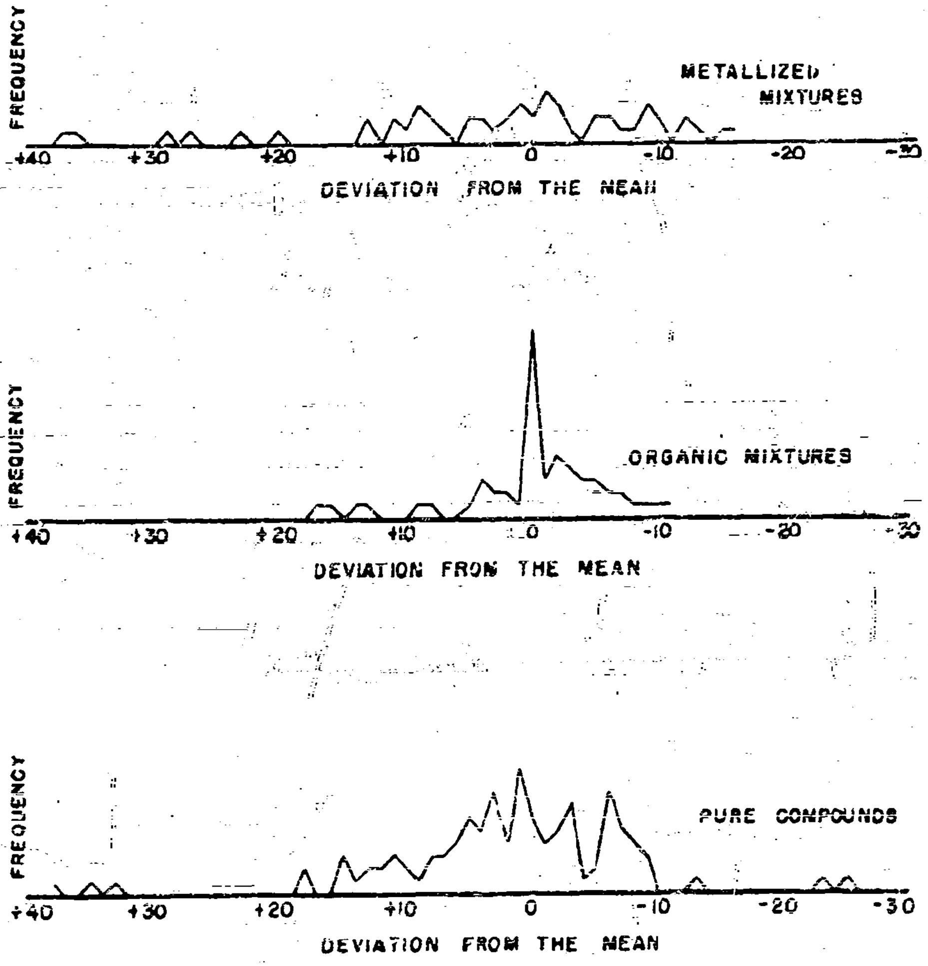

FIGURE 83
STATISTICAL DISTRIBUTION OF DEVIATIONS FROM THE MEAN COMPARING BALLISTIC MORTAR AND nRT FOR EXPLOSIVE SUBSTANCES

Table 143

Properties of Selected Pure Organic Compounds

No.	Name	O.B.	Calculated Q_c Kcal/mol	Q_e	Calc. Expl. T, °K	Power, TNT Calc.	B.M.	Dev.
6	4-Hydroxytetrahydropyran-3,3,5,5-tetramethanol pentanitrate	-30.4	1040.1	467.7	3651	129	137	+ 8
22	HMX	-21.6	635.1	365.8	4271	151	150	- 1
23	RDX	-21.6	477.6	275.6	4285	152	150	- 2
24	Hexahydro-1,3,5-trinitroso-s-triazine (R-salt)	-65.1	518.9	144.4	2930	[illegible]	[illegible]	[illegible]
25	2,4,6,8-Tetranitro-2,4,6,8-tetrazanonane-1,9-diol diacetate	-52.3	1149.5	255.9	2235	96	83	-13
26	~~2,4,6-Trinitro-2,4,6-triazaheptane-1,7-diol~~ diacetate	-68.7	992.6	166.4	1840	82	120	+38
33	Guanylurea perchlorate	-16.2	279.9	143.2	2798	99	92	- 7
35	Diethanolnitramine dinitrate	-26.7	552.0	282.6	3920	143	140	- 3
37	Diethylene glycol dinitrate	-40.8	503.7	176.8	3014	121	127	+ 6
41	2,2-Dimethyl-1,3-propanediol dinitrate	-74.2	658.6	117.9	2375	103	108	+ 5
42	1,3-Dinitramino-2-propanol nitrate	-17.8	456.2	289.5	4236	148	142	- 6
43	2,4-Dinitroaniline	-91.7	701.3	103.7	2110	81	88	+ 7
44	2,4-Dinitroanisole	-96.9	788.2	92.1	1805	72	87	+15
45	m-Dinitrobenzene	-95.2	678.8	107.4	2362	86	86	0
47	2,2-Dinitro-1-butanol	-60.2	514.5	72.6	1672	80	94	+14
54	3a,6a-Dimethyl-1,6-dinitroglycoluril	-61.5	744.7	110.6	1765	78	71	- 7
58	[illegible]	-34.8	472.3	145.4	2687	103	116	+13
63	N,N'-Bis(2-hydroxyethyl)-N,N'-dinitrooxamide dinitrate	-18.0	672.7	403.3	4002	128	135	+ 7
65	1,1-Dinitroethane	-26.7	267.2	132.6	3357	144	138	- 6
66	3,3-Dinitro-2-[illegible]	-27.3	375.5	176.8	3130	130	129	- 1
68	1,6-Dinitroglycoluril	-27.6	455.0	185.6	3244	110	101	- 9
71	2,4-Dinitrophenol	-78.2	611.8	86.7	1980	75	52	-23
74	2-(3,5-Dinitrophenyl)-2-nitro-1,3-propanediol dinitrate	-40.3	989.2	354.3	3646	127	126	- 1
75	[illegible]	-72.7	616.6	117.3	2275	114	107	- 7
76	1,1-Dinitropropane	-59.7	412.2	95.2	2435	111	103	- 8
77	2,2-Dinitro-1-propanol	-42.6	377.3	117.8	2722	111	122	+11
81	2,5-Bis(hydroxymethyl)-2,5-dinitro-1,6-hexanediol tetranitrate	-21.4	956.6	554.6	4167	139	147	+ 8
82	2,6-Bis(hydroxymethyl)-2,6-dinitro-1,7-heptanediol tetranitrate	-31.2	1104.4	496.3	3711	134	137	+ 3
84	2,4-Dinitrotoluene	-114.2	823.9	101.7	1965	76	71	- 5
88	2,4,6,8-Tetranitro-2,4,6,8-tetrazanonane-1,9-diol dinitrate	-3.7	736.2	658.9	4980	151	155	+ 4
89	Dipentaerythritol hexanitrate	-27.5	1187.7	541.6	3776	132	144	+12
92	Dulcitol hexanitrate	-7.1	637.1	637.1	4754	130	145	+15
93	Erythritol tetranitrate	+5.3	440.9	440.9	4848	133	151	+18
95	Ethylenediamine dinitrate	-25.0	359.8	167.6	2802	119	114	- 5
96	Ethylenedinitramine, EDNA	-32.0	358.4	166.2	3570	146	139	- 7
102	Ethyl nitrate	-61.5	294.0	73.0	2530	122	123	+ 1
111	1-Monolactin trinitrate	-29.4	463.7	233.4	2245	117	114	- 3
113	1-Monopicrin dinitrate	-31.6	358.6	196.2	3750	126	120	- 6
115	Guanidine perchlorate	-5.0	221.3	187.6	4037	133	124	- 9
116	1-Guanyl-3-nitrourea	-38.1	282.2	61.3	1755	73	75	+ 2
119	1,2,3,4,5,6-Benzenehexamethanol hexanitrate	-36.3	1341.5	533.4	3742	130	138	+ 8
125	2,2',4,4',6,6'-Hexanitrodiphenylamine	-52.8	1301.3	349.5	3379	121	115	- 6
128	2,2',4,4',6,6'-Hexanitrodiphenyl ether	-47.3	1312.3	356.7	3621	116	113	- 3
130	N,N'-Dipicrylethylenedinitramine	-44.3	1575.2	517.4	3674	129	123	- 6
135	1,3-Dipicrylurea	-53.1	1254.7	306.5	2735	101	76	-25
136	Hexanitroethane	+42.7	173.3	173.3	2641	[illegible]	[illegible]	[illegible]

Table 14 (continued)

Properties of Selected Pure Organic Compounds

No.	Name	ΔH_f	Calculated Q_v Kcal/mol	Calculated Q_e Kcal/mol	Calc. Expl. T, °K	Power, TNT Calc.	Power, TNT B.M.	Power, TNT Imp.
152	Mannitol hexanitrate	+7.1	637.1	637.1	4794	130	136	+6
163	N-Methylethylenedinitramine	-58.5	506.3	131.8	2615	126	120	-6
165	1,2,3-Butanetriol trinitrate	-16.6	492.5	324.1	4368	143	140	-3
168	2-Methyl-2-nitro-1,3-propanediol dinitrate	-24.8	601.3	265.6	3943	138	136	-2
170	N-Ethylethylenedinitramine	-58.5	505.3	130.8	2600	125	118	-7
180	2-Nitroethanol nitrate	-11.8	457.3	190.0	4470	144	142	-2
181	Nitroglycerin	+3.5	345.6	345.6	4835	140	140	0
182	Nitroguanidine	-30.8	187.8	63.0	2255	95	104	+9
185	Nitromethane	-39.3	257.2	61.6	3116	134	134	0
187	N-Methyl-N-nitroglycolamide nitrate	-22.3	360.0	191.7	3724	127	133	+6
189	2-Nitro-2-(m-nitrophenyl)-1,3-propanediol dinitrate	-57.8	1040.0	241.4	2535	112	114	+2
192	ω, ω, m-Trinitrotoluene	-74.0	786.8	145.5	2516	97	100	+3
194	2-Nitro-1-(o-nitrophenyl)ethanol nitrate	-77.8	921.2	155.1	2324	95	99	+4
200	Nitrourea	-7.6	113.4	79.8	2810	94	105	+11
202	N-Methylethanolnitramine nitrate	-43.6	454.1	265.8	3248	138	137	-1
207	Pentaerythritol tetranitrate	-10.1	584.7	450.0	[illegible]	[illegible]	145	+4
208	2,3,4,5,6-Pentanitroaniline	-15.1	410.4	408.4	4997	137	142	+5
216	Picric acid	-45.3	601.[illegible]	168.6	3130	108	[illegible]	+1
228	2-Hydroxy-1,1,3,3-cyclohexanetetramethanol pentanitrate	-44.9	1227.1	410.0	3206	126	127	+1
229	2,2,6,6-Tetrakis(hydroxymethyl)cyclohexanone tetranitrate	-56.3	1184.6	281.2	2575	108	114	+6
230	2-Hydroxy-1,1,3,3-cyclopentanetetramethanol pentanitrate	-35.3	1595.5	450.7	3640	133	151	+18
231	2,2,5,5-Tetrakis(hydroxymethyl)cyclopentanone tetranitrate	-45.8	1043.5	322.5	3032	117	122	+5
232	2,2-bis(nitraminomethyl)-1,3-propanedinitramine	-41.0	812.6	301.4	3247	137	129	-8
233	2,3,4,6-Tetranitroaniline	-32.2	641.5	271.1	4035	127	121	-8
240	Tetranitromethane	+49.0	78.1	78.1	2253	58	109	+51
241	1,3,6,8-Tetranitronaphthalene	-72.7	1066.0	224.4	2932	100	101	+1
243	N-Methyl-N,2,3,4,6-pentanitroaniline	-28.9	760.7	376.6	4432	140	141	+1
248	Tetrakis(2-hydroxyethyl)ammonium pentanitrate	-33.0	1053.0	456.8	3490	133	138	+5
253	Tetryl	-47.3	809.4	251.8	3480	127	130	+3
258	1,2-Propanedinitramine	-58.5	504.3	130.2	2592	124	116	-8
261	2-Ethyl-2-(hydroxymethyl)-1,3-propanediol trinitrate	-65.0	950.4	200.2	2410	112	117	+5
263	2-(Hydroxymethyl)-2-methyl-1,3-propanediol trinitrate	-34.5	836.3	270.9	3558	134	136	+2
265	2-Ethyl-2-(hydroxymethyl)-1,3-propanediol	-50.5	782.7	234.[illegible]	2935	124	127	+3
270	Picramide	-56.1	672.4	153.4	2797	107	110	+3
271	2,4,6-Trinitroanisole	-62.5	751.7	135.5	2366	94	106	+12
274	1,3,5-Trinitrobenzene	-56.3	647.[illegible]	157.3	3102	115	111	-4
275	2,4,6-Trinitrobenzoic acid	-46.7	644.4	144.2	2548	87	98	+11
276	2,4,6-Trinitrobenzyl nitrate	-38.9	750.0	278.7	3385	130	127	-3
277	2,4,6-Trinitro-m-cresol	-62.5	745.6	130.4	2285	93	96	+3
282	3-Ethyl-2,2,3-trinitropentane	-98.6	[illegible]	92.0	1625	75	82	+7
[illegible]	2,4,6-Trinitro-m-xylene	-103.5	1080.5	137.3	1735	80	84	+4
285	2-Methyl-2,3,3-trinitrobutane	-65.7	674.6	136.7	2318	108	106	-2
291	3-Methyl-2,2,3-trinitropentane	-83.2	819.1	98.8	1660	85	86	+1
29[illegible]	1,3,8-Trinitronaphthalene	-100.3	[illegible]	174.5	[illegible]	82	83	+1
294	2,4,6-Trinitrophenetole	-77.8	702.2	136.1	2102	86	80	-6
305	2-(N,2,4,6-Tetranitroanilino)-1-butanol nitrate	-57.4	1207.3	303.8	[illegible]	120	117	-3
307	2-(N,2,4,6-Tetranitroanilino)ethanol nitrate	-35.4	911.1	377.4	[illegible]	135	133	-2

Table 143 (continued)

Properties of Selected Pure Organic Compounds

No.	Name	O.B.	Calculated Q_C Kcal/mol	Calculated Q_E Kcal/mol	Calc. Expl. T. °K	Power, %TNT Calc.	Power, B.M.	Power, Dev.
308	2-(Hydroxymethyl)-2-(N,2,4,6-tetranitroanilino) 1,3-propanediol trinitrate	-21.9	1106.4	635.0	4551	140	143	+ 3
310	Styphnic acid	-45.7	557.1	186.7	3205	103	108	+ 5
313	2,4,6-Trinitrotoluene	-74.0	[illegible]	[illegible]	[illegible]	100	100	0
318	2,4,6-Trinitro-m-xylene	-89.6	935.4	143.1	2206	88	88	0
319	1,1',1''-Tris(methylnitramino)trimethylamine	[illegible]	1607.6	[illegible]	3259	109	107	- 2
320	Urea nitrate	[illegible]	105.7	72.0	2163	[illegible]	92	+15
324	n-Propyl picrate	-91.5	1047.0	130.0	1845	[illegible]	87	+10
325	Allyl picrate	-86.2	1019.7	160.1	[illegible]	88	91	+ 3
326	2-Propynyl picrate	-80.9	1001.3	199.2	2840	102	99	- 3
327	Nitroform	+37.1	112.4	112.4	3280	90	125	+35
328	Methylenedinitramine, MEDINA	0.0	212.2	212.2	4898	158	158	0
329	N-Methyl-N,2,3,4,5-pentanitroaniline	-28.9	780.7	375.6	4432	140	134	- 6
331	1,3-Bis(2,2,2-trinitroethyl)urea	0.0	580.4	580.4	5128	140	144	+ 4
337	Bis(2,2,2-trinitroethyl)nitramine, BTNEN	+16.5	478.0	478.0	4649	126	139	+13
340	2,2,2-Trinitroethanol 4,4,4-trinitrobutyrate	+ 4.1	624.6	557.2	4975	135	136	+ 1
343	2,2,3,3-Tetranitrobutane	-20.2	504.2	302.2	4335	143	153	+10
384	1,2-Dinitroethane	-26.7	267.2	112.6	3720	136	127	- 9
570	2-Methyl-2,3,3-trinitropentane	-63.2	815.1	98.8	1660	85	86	+ 1

Table 14

Properties of Selected Explosives Mixtures

No.	Mixture and Composition Ratios	O.B.	Calculated Q_c Kcal/gm	Calculated Q_e Kcal/gm	Calc. Expl. T.°K	Power, %TNT Calc.	Power, %TNT B.M.	Power, %TNT Diff.
M-370	C-4 (Harrisite), RDX/Di-2-ethylhexyl sebacate/PIB/oil, 91/5.3/2.1/1.6	-45.9	486.4	167.5	3299	132	130	-2
M-401	Amatol. TNT/AN, 85/15	-59.9	546.3	117.3	2580	106	106	0
M-402	70/30	-45.8	387.5	115.5	2905	125	114	-1
M-404	55/45	-31.7	276.6	114.3	3192	122	122	0
M-405	50/50	-27.0	246.7	113.9	3280	113	123	0
M-406	40/60	-17.8	194.9	116.8	3515	128	128	0
M-407	30/70	-8.2	151.1	116.6	[illegible]	[illegible]	[illegible]	[illegible]
M-408	25/75	-3.5	132.0	117.9	3737	131	131	0
M-409	20/80	+1.2	114.2	114.2	3705	130	130	0
M-410	15/85	+5.9	97.5	97.5	3369	121	129	+8
M-411	10/90	+10.6	82.1	82.1	3033	111	125	+14
M-412	5/95	+15.3	67.7	67.7	2690	101	117	+16
M-419	EDNA/AN, 50/50	-2.9	116.8	150.5	3665	130	123	-7
M-420	45/55	-0.6	133.8	131.0	3560	131	126	-5
M-421	EDNA/TNT/AN, 20/20/60	-8.0	157.9	122.4	3530	139	134	-5
M-422	EDNA/RDX/AN, 35/30/35	-0.6	205.3	257.9	3666	135	138	+3
M-423	MAN/AN, 40/60	-1.6	152.0	102.2	3430	131	122	-9
M-430	Comp. A. RDX/Beeswax, 88/12	-57.6	737.5	190.0	2710	123	132	+9
M-431	91/9	-48.6	668.3	212.9	3090	132	135	+3
M-434	RDX/AN/Beeswax, 45.5/50/4.5	-24.2	209.3	94.5	4860	125	127	+17
M-436	RDX/TNT/Wax, 59.5/39.5/1.0	-46.4	673.9	807.8	3386	132	133	+1
M-437	Comp. C. RDX/Oil, 88/12	-60.1	554.9	64.3	2810	130	120	-10
M-438	DNT/TNT/NC/RDX/Wax, 12/2/2/79/5	-40.9	506.4	198.3	3590	147	143	-4
M-439	DNT/MNT/NC/RDX/TNT/Tetryl, 10/5/1/77/4/3	-41.8	561.8	206.0	3503	137	126	-11
M-440	Cyclotol. RDX/TNT, 30/70	-60.3	686.7	147.5	2905	117	120	+3
M-441	40/60	-53.0	665.0	183.2	3110	123	127	+4
M-442	50/50	-45.8	627.7	208.5	3418	132	126	-6
M-443	60/40	-42.6	602.0	214.8	3530	135	133	-2
M-444	70/30	-37.3	570.7	233.7	3718	140	135	-5
M-447	MAN/TNT, 45/55	-52.3	576.4	143.8	2579	107	109	+2
M-448	Ednatol. EDNA/TNT, 50/50	-53.0	521.2	137.8	2809	117	117	0
M-450	55/45	-50.9	500.0	139.7	2860	119	119	0
M-449	60/40	-48.8	480.0	140.3	2926	121	121	0
M-451	EL-389A. DNT/NG/TNT, 31.5/55/13.5	-44.0	575.9	193.7	3399	127	126	-1
M-452	EL-389B. DNT/NG/TNT, 28/60/12	-38.7	551.9	209.4	3606	130	127	-3
M-453	EL-389C. DNT/NG/TNT, 35/50/15	-49.3	599.5	178.3	3189	122	115	-7
M-454	Pivonite/EDNA, 50/50	-38.9	538.8	158.3	3165	126	130	+4
M-455	Pivonite/PETN, 50/50	-28.9	761.8	383.6	3643	132	132	0
M-456	Pivonite/RDX, 50/50	-33.7	[illegible]	[illegible]	[illegible]	135	[illegible]	-2
M-457	Pivonite/RDX, 53/47	-34.4	700.9	294.1	3626	134	135	+1
M-459	Methylite-25. NG/Dimethyl phthalate, 75/25	-40.6	546.6	179.9	3035	113	111	-2
M-460	Methylite-30. NG/Dimethyl phthalate, 70/30	-49.5	584.9	118.3	2595	102	102	0
M-463	Pentolite. PETN/TNT, 25/75	-59.3	757.5	166.7	2700	107	111	+4
M-466	50/50	-42.0	705.7	445.1	3475	127	126	-1
M-467	75/25	-30.1	650.6	334.1	4065	136	136	0
M-468	PEP-1. PETN/TNT/Oil, 21.3/63.7/15	-100.6	399.2	60.1	1950	89	108	+19
M-469	PEP-2. PETN/Oil, 86/14	-66.6	444.4	65.9	2820	123	115	-8
M-470	Picratol. PA/TNT, 52/48	-59.1	693.6	145.3	2588	103	100	-3
M-471	PTX-2. RDX/PETN/TNT, 28/44/28	-33.3	595.5	280.1	3062	138	138	0
M-472	PTX-1. RDX/Tetryl/TNT, 30/50/20	-45.0	652.9	430.7	3502	131	132	+1
M-474	PIPE, RDX/Oil, 81/19	-48.5	220.9	39.1	2280	112	[illegible]	-6
M-475	[illegible] RDX/Oil, 75/25	-47.7	[illegible]	50.1	2730	[illegible]	[illegible]	0
M-478	Tetrytol. Tetryl/TNT, 75/25	-54.0	804.4	213.7	3141	120	122	+2
M-484	DNT/NC/PETN/TNT/Dibutyl phthalate, 22.9/4/64.5/4.7/3.3	-42.5	664.6	427.6	3310	124	129	+5
M-485	DNT/NC/RDX/TNT/Dibutyl phthalate, 18.6/4.4/73.5/3.3/2.4	-53.8	556.5	172.4	3355	133	146	+13
[illegible]	DNT/NC/PETN/TNT, 16.7/[illegible]/[illegible]/5.5	-31.9	637.0	298.1	3371	137	139	-2

Table 145

Properties of Selected Metallized Explosive Mixtures

Mixture and Composition Ratios	Metal Oxide State	O.B.	Calculated Q_C	Q_E kcal/mole	Calc. Expl. T, °K	Power, Calc.	B.M.	Diff. %
Aluminized Comp. A RDX/Al/Wax, 73/18/9	solid	-51.7	373.9	169.3	5580	158	142	-10
	gas			159.1	5071	152		-9
Aluminized Ednatol. EDNA/TNT/Al	solid	-60.2	319.7	142.4	5056	135	130	-5
	gas			113.7	4177	125		+5
Tritonal. TNT/Al, 90/10	solid	-75.5	506.6	155.8	3961	118	124	+5
	gas			133.6	3492	110		+13
80/20	solid	-77.0	490.5	157.5	5175	108	117	+9
	gas			125.4	4250	104		+13
70/30	solid	-76.5	323.3	158.5	6117	76	105	+39
	gas			122.6	4935	85		+20
40/60	solid	-83.0	243.1	58.2	4549	28	49	
	gas			44.8	3634	34		
Minol (aluminized Amatol). TNT/AN/Al, 40.45/54.55/5	solid	+4.7	131.6	100.6	3870	129	130	+1
	gas			95.0	3670	126		+4
9/81/10	solid	+0.7	112.7	112.4	4557	139	136	-3
	gas			100.2	4415	133		+3
66.75/22.25/11*	solid	-54.7	335.3	117.2	[illegible]	137	122	-15
	gas			98.1	3?80	124		-2
67/22/11	solid	-55.0	337.7	117.6	3815	137	122	-15
	gas			98.5	[illegible]	124		-2
8.8/79.2/12	solid	+1.4	117.6	113.7	5594	115	136	+11
	gas			99.9	5037	133		+23
36/51/13	solid	-28.3	296.8	113.3	4670	145	133	-12
	gas			94.4	4082	135		-2
72.25/12.75/15	solid	-64.2	359.7	135.6	4480	130	117	-13
	gas			111.0	3790	119		-2
[illegible]	solid	[illegible]	220.8	113.6	4835	149	143	-6
	gas			91.2	4015	135		+8
40/42/18	solid	[illegible]	[illegible]	113.6	[illegible]	147	143	-6
	gas			91.2	4019	135		+8
40/40/20	solid	-39.4	222.0	113.7	5010	151	143	-5
	gas			89.9	4095	136		+7
Torpex. RDX/TNT/Al, 41.5/41.5/17	solid	-54.8	359.9	162.6	5182	142	133	-9
	gas			133.8	4286	132		+1
41.82/40.18/18*	solid	-54.8	361.8	162.5	5258	142	134	-8
	gas			133.0	4430	132		+2
42/40/18	solid	-54.7	[illegible]	162.9	5306	141	134	-7
	gas			133.1	4466	132		+2
HBX. RDX/TNT/Al/Desensitizer, 39.6/37.7/17.1/5.5	solid	-56.0	393.7	162.4	4860	135	126	-9
	gas			133.2	4480	125		0
RDX/TNT/Al/Wax, 41.16/39.20/17.64/2.00	solid	-61.2	370.2	161.2	5046	138	132	-6
	gas			131.7	4245	128		+4
RDX/TNT/Al/Vistanex, 39.90/38.00/17.10/5	solid	-66.5	390.6	158.4	4770	133	132	-1
	gas			139.5	4020	123		+9
RDX/TNT/Al/Vinsol, 37.80/36.00/16.20/10	solid	-78.2	432.3	153.8	4095	126	126	0
	gas			125.2	3625	116		+10
DNT Torpex. DNT/RDX/Al, 34/48/18	solid	-66.2	364.5	154.3	4951	134	133	-1
	gas			125.8	4168	125		+8
DBX. RDX/TNT/AN/Al, 21/40/21/18	solid	-43.9	275.8	128.7	4563	151	146	-5
	gas			103.2	4105	137		+9
Boratorpex. RDX/TNT/B, 48.6/46.4/5	solid	-55.9	379.8	138.1	3943	137	127	-10
	gas			115.7	3426	126		+1
47.1/44.9/8	solid	-50.4	321.6	141.9	4746	142	131	-11
	gas			117.5	3992	132		-1
46/44/10	solid	-64.7	395.9	128.5	4450	124	126	+2
	gas			99.8	3751	115		+11
43.5/41.5/15	solid	-73.4	253.6	150.9	6151	113	112	-1
	gas			113.6	5048	122		-10
41/39/20	solid	-78.3	229.0	116.9	3670	74	101	+37
B_2O_3	gas			50.2	1515	69		+46
$B + B_2O_3$	gas			47.4	1740	64		[illegible]

* Duplication of preceding composition; not included in statistical analysis.

Note: Ballistic mortar data for additional HBX-type explosives in (5) were noted too late for inclusion in this tabulation.

1. Organic Compounds

It will be noted that of the 111 pure compounds given in Table 143, only six display deviations from the mean greater than plus or minus 18, that is about three times the standard deviation which is commonly considered to include 99% of the deviation due to chance. These six which were excluded from the statistical analysis, are compound numbers 26, 71, 135, 136, 240 and 327. Data on these are summarized in Table 146.

Table 146
Pure Compounds Showing Large Differences Between Observed Ballistic Mortar and Calculated nRT Values

Compound		Power, % TNT			
No.	Name	O.B.	Calc.	B.M.	Dev.
26	2,4,6-Trinitro-2,4,6-triazaheptane-1,7-diol diacetate	-58.7	82	120	+38
71	2,4-Dinitrophenol	-78.2	75	52	-23
135	1,3-Dipicrylurea	-53.1	101	76	-25
136	Hexanitroethane	+42.7	75	108	+33
240	Tetranitromethane	+49.0	58	109	+51
327	Nitroform	+37.1	90	125	+35

Of these compounds, the large negative deviations for numbers 71 and 135 may possibly be explained by the fact that these were not actually the compounds measured or perhaps even that they did not detonate completely in the ballistic mortar. Compounds 136, 240 and 327 have large positive oxygen balances, +42.7, +49.0 and +37.1, respectively, a fact which gives an explanation for the large positive discrepancies found, for it may be reasonably assumed that the excess oxygen reacts with the detonator which itself has a negative oxygen balance. This explanation has been substantiated by two recent ballistic mortar measurements made by the Bureau of Mines. Tetranitromethane 240, and bis(trinitroethyl)trinitramine (...), 37, were remeasured using in place of the usual electric detonator, a modified No. 6 type detonator free of a combustible seal. The explosive charge of this detonator consisted of 0.29 gram of PETN base charge, and 0.41 gram of 75-25 DDNP-$KClO_4$ primary charge.

The ballistic mortar value for TNM was thereby reduced from 141 to 109% TNT; for HOX from 155 to 139% TNT. Thus the deviation between measured and calculated power for HOX, the only other compound of high positive oxygen balance, was reduced to +13, or within the range of accepted error. The large difference still existing between the measured and calculated values for TNM may well be explained by other thermodynamic characteristics of this material (see page 476). The deviation of +38 for compound number 26 can not be explained except to state that there is the possibility that the compound measured was not what it was thought to be.

Although it does not appear warranted to make any generalizations concerning a correlation between measured and calculated values and the probable degree of purity of the compound or the accuracy of measurement, it should be pointed out that deviations between measured and calculated values are at a minimum for compounds which are best known and hence probably most nearly pure. Among such compounds are HMX (22), RDX (23), ethyl nitrate (102), nitroglycerin (181), nitromethane (185), PETN (207), picric acid (216), Tetryl (253) and MEDINA (328).

2. Explosives Mixtures

An even better correlation is indicated for the organic mixtures, as shown in Table 144 and Figure 81. This may be due to the fact that the mixtures are generally made up of the more common, and hence better evaluated, compounds such as TNT, RDX, PETN and EDNA. As in the case of pure compounds, there may be even the effect of positive oxygen balance (M-410, 411 and 412) upon the ballistic mortar values.

In Figure 84, there are plotted the measured and calculated values for a series of Cyclotols (RDX/TNT). This figure illustrates one of the uses this calculation system has, that is, an independent check on observed values. Here it appears that there are discernable errors in the measured values for there is no explanation for the rather erratic behavior indicated in the range of 40 to 65% RDX (M-441, 442 and 443). Rather, it is to be expected that the power of this mixture increases as the per cent of RDX is increased as shown by the calculated powers.

3. Metallized Mixtures

The calculation of metallized mixtures is attended by added complications, including gross assumptions as to the products formed, whether the inorganic oxides assumed to be formed are gaseous or solid, and finally a general insufficiency of thermodynamic data. As pointed out previously, the metals were assumed to oxidize completely (i.e., to Al_2O_3, B_2O_3 or MgO). All calculations were made for both solid and gaseous metal oxides and as will be seen in Table 145 and Figure 82, the corresponding "solid" and "gaseous" values generally lie above and below the line, respectively. Hence, it would appear that a true correlation lies between

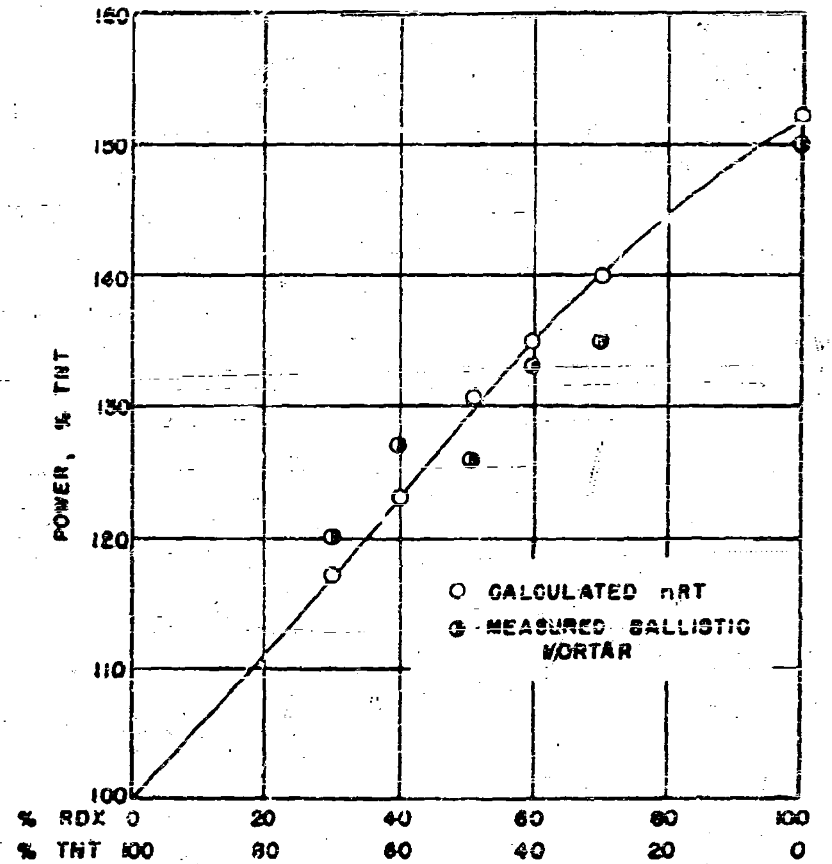

FIGURE 84

COMPARISON OF BALLISTIC MORTAR AND CALCULATED nRT FOR CYCLOTOLS (RDX/TNT)

the "solid" and "gaseous" values. This is borne out by the -0.8 average deviation shown when the "solid" and "gaseous" figures are considered together (Figure 83).

Because of the assumptions which had to be made and because some of the temperatures calculated are apparently out of the range which can be handled confidently by such a simplified system, it is not claimed that the calculated temperatures and energies for metallized mixtures represent the true values. They are, however, generally of the same relative order of magnitude as measured by the ballistic mortar and the spherical lead block. (Tables 145 and 147).

There is some reason to believe that the power values for metallized mixtures as measured in the ballistic mortar and lead block to date may be somewhat in error as illustrated by Figure 85. There it is shown that the ballistic mortar and cylindrical lead block measurements for a series of Tritonals (TNT/Al) disagree as to the optimum per cent of aluminum, that is, the location of the peak of the curve. Calculated powers are somewhat lower than measured powers, but again there is general agreement between the observed ballistic mortar and calculated nRT as to the peak and the overall shape of the curve.

Since it is generally believed that the ballistic mortar and the spherical lead block measure shock power, as contrasted to blast power, the use of these two test methods, and hence the nRT calculation method, cannot be considered as a final means of evaluating metallized explosives.

4. Correlation of Spherical Lead Block Measurements and nRT

The new type spherical lead block will be discussed in detail in a forthcoming report. It is sufficient to point out here that results are based upon an equivalent weight, i.e., on a weight of explosive required to give an expansion in the block equivalent to a specified expansion for TNT. The power measurements resulting from the spherical lead block correlate directly with nRT calculations and therefore also with ballistic mortar values. This is shown in Table 147.

Taking all the values given in Table 147, the average deviation is calculated to be +0.1 and the standard deviation 4.9. Thus the correlation (indicated to date on twenty-nine compounds) of calculated nRT with spherical lead block measurements is as good as with ballistic mortar measurements.

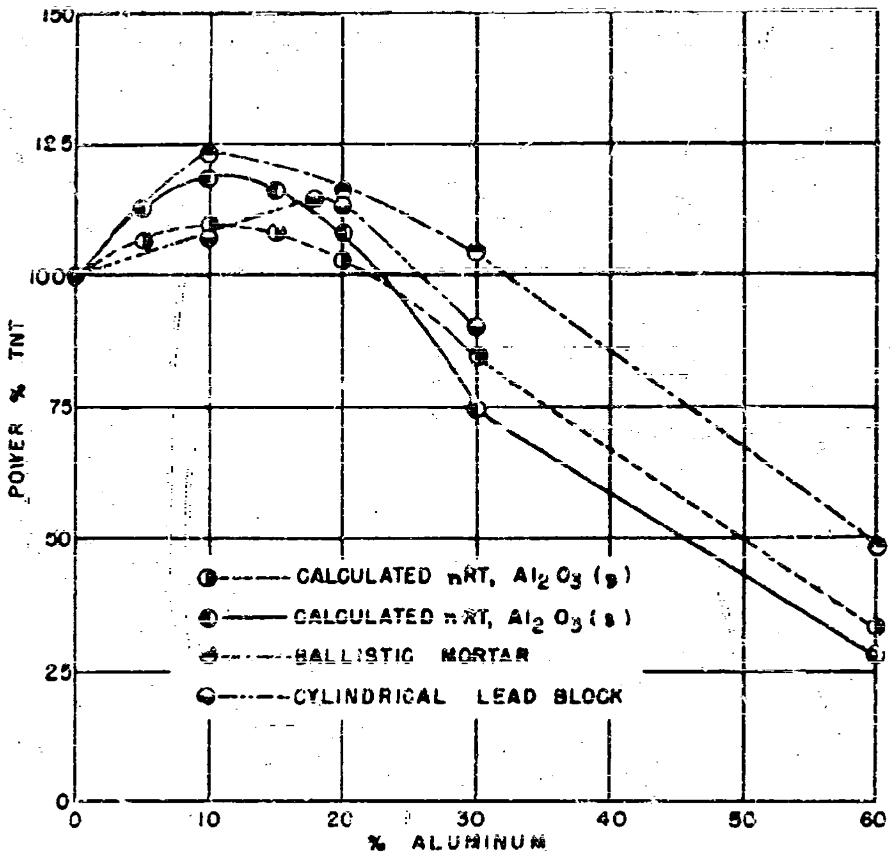

FIGURE 85

COMPARISON OF CALCULATED nRT, BALLISTIC MORTAR AND SPHERICAL LEAD BLOCK FOR TRITONALS (TNT/AL)

Table 147
Correlation Between Calculated nRT and Spherical Lead Block Measurements

	Explosive Compound or Mixture	Al_2O_3 State	Power, % TNT Calc.	Lead* Block	Dev.	B.M.
	Pure Compounds					
22	HMX		151	146	- 5	150
23	RDX		152	149	- 3	150
182	Nitroguanidine		95	98	+ 3	104
253	Tetryl		127	124	- 3	130
310	Styphnic acid		103	102	- 1	108
313	2,4,6-Trinitrotoluene		100	100	0	100
328	Methylenedinitramine, MEDINA		158	155	- 3	158
337	Bis(2,2,2-trinitroethyl)nitramine, HOX		125	128	+ 3	139
342	5-Amino-1H-tetrazole		96	n.d.	-	-
352	Hydrazine nitrate		122	121	- 1	-
956	1-Amino-3-nitroguanidine		113	113	0	-
	Organic Mixtures					
	TNM/TNT, 56/44		152	160	+ 8	-
	RDX/TNM, 77/23		156	153	- 3	-
	HMX/HOX, 43.3/56.7		153	152	- 1	-
	HOX/TNT, 81.8/18.2		148	153	+ 5	-
	MEDINA/TNT, 80/20 (cast)		151	150	- 1	-
	MEDINA/TNT/Tetryl, 80/10/10		153	147	- 6	-
	MEDINA/Tetryl, 80/20		153	152	- 1	-
	MEDINA/Styphnic acid		149	151	+ 2	-
	RDX/Hydrazine nitrate, 55/45		146	150	+ 4	-
	RDX/TNT, 51.21/48.79		130	124	- 6	-
	Metallized Explosives					
	HOX-2H	solid	61	59	- 2	-
		gas	60		- 1	
	Torpex II, RDX/TNT/Al, 42/40/18	solid	141	144	+ 3	134
		gas	132		+12	
	Torpex II/Nitroguanidine, 61.17/38.83	solid	139	131	- 8	-
		gas	126		+ 5	
	Torpex II/Nitraminoguanidine, 57.92/42.08	solid	145	134	-11	-
		gas	132		+ 2	
	Aluminized MEDINATOL. MEDINA/TNT/Al, 76/19/5	solid	156	152	- 4	-
		gas	152		0	
	72/18/10	solid	160	157	- 3	-
		gas	153		+ 4	
	68/17/15	solid	163	163	0	-
		gas	154		+ 9	
	64/16/20	solid	164	163	- 1	-
		gas	155		+ 8	

* New-type spherical lead block.

5. Application to New Compounds and Mixtures

It is believed, however, that this simplified system has a more important application in predicting the relative power of pure compounds or mixtures as they would be measured by the ballistic mortar. A number of new - unusual compounds and mixtures which have been proposed as high explosives have been calculated. A few typical ones are given in Table 148 to illustrate the application of the method for calculating heats of combustion (Section XVI) and the power method here described.

Table 148
Properties of Selected High-Energy Compounds

Name	O.B.	Calculated Q_C^X Kcal/mol	Q_E^V	T, °K	Calc. % TNT
5-Trinitromethyl-1H-tetrazole	+12.0	267.7	267.7	6070	164
1,1,2,2-Tetranitroethylbis(5-azo-1H-tetrazole)	- 3.4	670.5	603.1	5849	168
1,1,1,6,6,6-Hexanitro-2,4-hexadiyne	0.0	698.0	698.0	7390	186
1,1,1,4,4,4-Hexanitro-2-butyne	+19.8	655.0	655.0	7750	188

It is recognized that none of the compounds listed in Table 148 have been synthesized and perhaps are not practical explosives, but they point up the need for examining certain structural groups, for example, -C≡C- and the tetrazole ring, which would be desirable from an energy point of view.

It is expected that this system will be extended to sulfur-containing compounds, to some halogenated compounds, and perhaps to mixtures containing metals other than those covered to date.

D. Method of Calculation

A form devised to standardize and expedite the nRT calculations is shown as Figures 86 and 87, the obverse and reverse sides, respectively. The following discussion of procedure is presented in terms of a typical step-by-step calculation for compound number 23, RDX, Figures 86 and 87.

It will be noted that the reverse side contains a small table for calculating the heat of combustion from the values of a' and b', as given in Section XVI of this report (see Table 60). These values are inserted

for the various groups present and Q_c^p (H_2O liquid) calculated from the general equation

$$Q_c^p \text{ (H}_2\text{O liquid)} = a' + x\Sigma b'.$$

Having calculated this Q_c^p (H_2O liquid) for the compound, there is added the value for ΔnRT to correct the value at constant pressure to heat of combustion at constant volume, Q_c^v. These values of 504.7 and 507.4 are then transferred to the "Calc." Q_c^p and Q_c^v lines on the front side of the sheet. From the value of 507.4 is subtracted the quantity (3.0 x 9.927) to convert to H_2O gas (See Table 140). From this value for heat of combustion at constant volume are then subtracted the energies required to burn any C to CO_2, CO to CO_2 and H_2 to H_2O. Thus, in the case of RDX, the quantity (3 x 67.341) is subtracted from the value of 477.6 to obtain the heat of explosion at constant volume in kcal/mol. The next step involves a series of iterations to arrive at an explosion temperature. This is done by assuming a temperature and setting down on the form the specific heats of the detonation products at this temperature as obtained from Table 149. The summation of the products of these specific heats and the number of moles of each gas present is then divided into the heat of explosion, multiplied by 1000 (to convert from kilogram calories to calories since the specific heats are given in the latter units) and added to 298, the base temperature, to give an approximate temperature. The true temperature lies between these approximate and assumed temperatures. The system is repeated until there results a final calculated temperature corresponding to the assumed temperature. This temperature is next inserted in the nRT equation along with the value for n, the total moles of gas formed, which has been obtained from the detonation equation. (See assumption page 580). The units for nRT thus found are kcal/mol. Subsequent conversions are made to kcal/kg and then to ft lbs/gram. The latter, when divided by the corresponding figure of 701.0 for TNT and multiplied by 100, results in an nRT product expressed in terms of per cent TNT.

There is provided on this form a space for calculating the molar and weight oxygen balances, two parameters often required in evaluating a high explosive.

In the case of organic mixtures, it has been found desirable to base all calculation on a total quantity equivalent to one mole of the mixture. Figures 88 and 89 give an example of this type of calculation illustrating the mixture of 60/40 EDNA/TNT (Ednatol). By dividing the weight per cent by the molecular weight of each of the components, a molar

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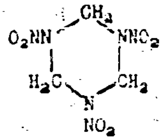
CALCULATION OF POWER BY THE NRT METHOD

Structural Formula



Name RDX

Number 23 Molecular Weight 222.13

Oxygen Needed 3.0 atoms/mol cpd

Oxygen Balance -21.6 gm O_2/100 gm cpd

Detonation $C_3H_6N_6O_6$ → $3\ CO + 3\ H_2O + 3\ N_2$

Σn = 9 mols gas/mol compound

Q_C^v = 477.6 Kcal/mol (H_2O gas)

Q_E^v = 275.6 Kcal/mol (H_2O gas)

Obs. Q_C^p = 501.8 Kcal/mol (H_2O liq.)

Q_C =

Calc. Q_C^p = 504.7 Kcal/mol (H_2O liq.)

Q_C^v = 507.4

Thermodynamic Data Reference:

No. Mols	Product	Average C_v (cal/mol/°K) from 298° to Assumed Flame Temperature: 4190 °K	4290 °K	°K	°K	°K	°K	°K
	CO_2							
3	H_2O	10.00	10.06					
3	CO	6.50	6.51					
3	N_2	6.45	6.47					
	H_2							
	O_2							
	C							
ΣnC_v		68.85	69.12					
$T = 298 + \frac{Q_E}{\Sigma nC_v} \times 10^3$		4301	4285					

$F = R \cdot T \cdot \Sigma n = 1.987 \times 4285 \times 9.0 \times 10^{-3}$

= 76.63 Kcal/mol

= 345.0 Kcal/Kg

= 1065.0 ft lbs/g (3.087 ft lbs = 1 cal)

= ____ / ____ (____)

Calc. Power $\frac{1065.0}{701.0}$ = 152 % TNT

Obs. Power B. M. = 150 % TNT (In Mines)

Equiv. Power, Lead Block = 149 % TNT ( )

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Figure 87

Compound Number 23

Calculation of Heat of Combustion

Structural Group No.	Name	a'	b'
1	Paraffin	5.7	52.08
2	Nitramine (s)	285.9	+.81
3	Sec. Amine (1)	54.9	-.12

Total 346.5
$\Sigma b'x$ 158.2
Q_c^p (H_2O liq) 504.7
ΔnRT 2.7
Q_c^v (H_2O liq) 507.4

$x = 3.0$

$\Delta n = -\frac{H}{4} + \frac{2N + 2\,O}{4}$

$\Delta n = \frac{-6 + 12 + 12}{4}$

$\Delta nRT = 4.5 \times 0.5923$

* * * * * * *

Other Calculations and Notes

C	H	N	O	

Case No. 56247
Date 12/26/51 By CRH

Figure 88

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CALCULATION OF POWER BY THE nRT METHOD

Structural Formula

60/40
0.3997/0.1761

Name Ednatol
EDNA/TNT

Number [illegible] Molecular Weight 173.67

Oxygen Needed +5.2935 atoms/mol cpd

Oxygen Balance -48.77 gm O_2/100 gm cpd

Detonation 0.6942 $C_2H_6N_4O_4$ 0.3058 $C_7H_5N_3O_6$ $\longrightarrow$ 3.5290 CO + 1.0826 H_2O + 1.7645 H_2 + 1.8471 N_2

Σn = 8.2232 mols gas/mol compound

Q_C = 480.2 Kcal/mol (H_2O gas)

Q_E = 140.9 Kcal/mol (H_2O gas)

Obs. Q_C = ______ Kcal/mol (H_2O liq.)

Q_C = ______

Calc. Q_C = ______ Kcal/mol (H_2O liq.)

Q_C = ______

Thermodynamic Data Reference: ______

No. Mols	Product	Average C_v (cal/mol/°K) from 298° to Assumed Flame Temperature 2900 °K	°K	°K	°K	°K	°K	°K
	CO_2							
1.0826	H_2O	9.17						
3.5290	CO	6.27						
1.8471	N_2	6.19						
1.7645	H_2	5.77						
	O_2							
	C							
ΣnC_v		53.56						
$T = 298 + \frac{Q_E}{\Sigma nC_v} \times 10^3$		2929						

$F = R \cdot T \cdot \Sigma n$ = 1.987 x 2925 x 8.2232 x 10^{-3}

= 47.79 Kcal/mol

= 275.2 Kcal/Kg

= 849.5 ft lbs/g (3.087 ft lbs = 1 cal)

= ______/______ (______)

Calc. Power $\frac{849.5}{701.0}$ = 121 % TNT

Obs. Power B. M. = 121 % TNT (Ref. (5))

Equiv. Power, Lead Block = ______ % ______ (______)

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Figure 89

Compound Number M-449

Calculation of Heat of Combustion

Structural Group No.	Structural Group Name	a'	b'

Total ______
$\Sigma b'x$ ______
Q_c^p (H_2O liq) ______
ΔnRT ______
Q_c^v (H_2O liq) ______

x = ______

$\Delta n = -\frac{H}{4} + \frac{2N + 2O}{4}$

Δn = ______

ΔnRT = ______ x 0.5923

* * *

Other Calculations and Notes

C	H	N	O	
1.3884	4.1652	2.7768	2.7768	
2.1406	1.5290	0.9174	1.8348	
3.5290	5.6942	3.6942	4.6116	
	2.8471	1.8471		

1.0826 H_2O
1.7645 H_2

Case No. 58247
Date 2-27-52 By RAL

Figure 90

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SECURITY INFORMATION

CALCULATION OF POWER BY THE nRT METHOD

Structural Formula

42/40/18
0.1891/0.1761/0.6674

Name Torpex II
RDX/TNT/Al

Number ______ Molecular Weight 96.84

Oxygen Needed +3.3092 atoms/mol cpd

Oxygen Balance -54.67 gm O_2/100 gm cpd

0.1831 $C_3H_6N_6O_6$
0.1705 $C_7H_5N_3O_6$
Detonation 0.6464 Al → 1.152 CO + 0.5908 C + 0.9756 H_2 + 0.8050 N_2
+ 0.3232 Al_2O_3

Σn = 2.9326 (3.2558) mols gas/mol compound

Q_C = 351.6 Kcal/mol (H_2O gas)   Obs. Q_C = ______ Kcal/mol (H_2O liq.)

Q_C = ______

Q_E = 162.7 (133.1)* Kcal/mol (H_2O gas)   Calc. Q_C = ______ Kcal/mol (H_2O liq.)

Thermodynamic Data Reference: ______ Q_C = ______

No. Mols	Product	Average C_v (cal/mol/°K) from 298° to Assumed Flame Temperature 5100 °K	5300 °K	(4530) °K	(4480) °K	°K	°K	°K
	CO_2							
	H_2O							
1.1520	CO	6.61	6.63	(6.54)	(6.54)			
0.8050	N_2	6.57	6.60	(6.50)	(6.49)			
0.9756	H_2	6.42	6.46	(6.30)	(6.29)			
	O_2							
0.5908	C	6.20	6.16	(5.92)	(5.92)			
0.3232	Al_2O_3	29.68	29.70	(29.53)	(29.52)			
ΣnC_v		32.36	32.49	(31.96)	(31.93)			
$T=298+\frac{Q_E}{\Sigma nC_v}\times10^3$		5326	5306	(4463)	(4466)			

$$F = R\cdot T\cdot\Sigma n = 1.987 \times \underset{5306}{(4468)} \times \underset{2.9326}{(3.2558)} \times 10^{-3}$$

= (28.90) 30.92 Kcal/mol

= (298.5) 319.3 Kcal/Kg

= (921.5) 985.7 ft lbs/g (3.087 ft lbs = 1 cal)

= ______ ______/______(______)

* Numbers in ( ) for Al_2O_3 (g)

Calc. Power $\frac{(921.5)\ 985.7}{701.0}$ = (132) 141 % TNT

Obs. Power B. M. = 134,138 % TNT (Ref. (5))
Equiv. Power, Lead Block = 143, 145 % TNT (______)

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Figure 91

Compound Number ______________

Calculation of Heat of Combustion

Structural Group No.	Structural Group Name	a'	b'

Total ______
$\Sigma b'x$ ______
Q_c^p (H_2O liq) ______
ΔnRT ______
Q_c^v (H_2O liq) ______

x = ______________

$$\Delta n = -\frac{H}{4} + \frac{2N + 2O}{4}$$

Δn = ______________

ΔnRT = ________ x 0.5923

* * * * * * * *

Other Calculations and Notes

C	H	N	O	Al
0.5423	1.0986	1.0986	1.0986	
1.1935	0.8525	0.5115	1.0230	0.6464
1.7428	1.9511	1.5101	2.1216	0.6464
1.1520	.9756	.8050		.3232

.5908 C

Case No. 58247
Date 1-2-52 By BAL

Table 149

Average C_v Over Range from 298 °K to T
(calories/mole/°K)

T, °K	CO_2	H_2O	CO	N_2	H_2	O_2	C(s)	HCl	Al_2O_3	B_2O_3	MgO
1000	9.40	6.88	5.40	5.33	5.06	5.75	4.02	5.15	25.71	26.55	11.07
10	9.43	6.89	5.41	5.33	5.06	5.76	4.04	5.16	25.75	26.63	11.10
20	9.44	6.90	5.42	5.34	5.06	5.76	4.05	5.16	25.81	26.70	11.12
30	9.47	6.92	5.43	5.35	5.06	5.77	4.06	5.17	25.86	26.76	11.14
40	9.49	6.94	5.43	5.36	5.07	5.78	4.07	5.17	25.90	26.80	11.16
50	9.52	6.95	5.44	5.36	5.07	5.79	4.09	5.18	25.94	26.86	11.19
60	9.54	6.96	5.45	5.37	5.07	5.80	4.10	5.18	25.99	26.90	11.21
70	[illegible]	[illegible]	5.46	5.38	[illegible]	5.80	4.12	5.19	26.02	26.95	11.24
80	9.58	7.00	5.47	5.39	[illegible]	5.81	4.13	5.19	26.06	[illegible]	11.26
90	9.60	7.01	5.47	5.39	5.08	5.82	4.14	5.20	26.10	27.04	11.28
1100	9.62	7.03	5.48	5.40	5.08	5.83	4.16	5.20	26.13	27.07	11.30
10	9.64	7.04	5.49	5.41	5.09	5.83	4.17	5.21	26.17	27.10	11.33
20	9.66	7.06	5.50	5.42	5.09	5.84	4.18	5.21	26.20	27.14	11.35
30	9.68	7.07	5.50	5.42	5.10	5.85	4.20	5.22	26.24	27.18	11.37
40	9.70	7.08	5.51	5.43	5.10	5.86	4.21	5.22	26.26	27.22	11.40
50	9.72	7.10	5.52	5.44	5.10	5.86	4.23	5.23	26.30	[illegible]	[illegible]
60	9.74	7.11	5.52	5.44	5.11	5.87	4.24	5.23	26.32	27.28	11.44
70	9.76	7.13	5.53	5.46	5.11	5.88	4.25	5.24	26.36	27.31	11.46
80	9.78	7.14	5.54	5.46	5.11	5.89	4.26	5.24	26.38	27.35	11.48
90	9.80	7.16	5.55	5.47	5.12	5.89	4.28	5.25	26.42	27.38	11.50
1200	9.82	7.17	5.55	5.47	5.12	5.90	4.30	5.26	26.45	27.41	11.53
10	9.84	7.19	5.56	5.48	5.12	5.90	4.31	5.26	26.48	27.44	11.55
20	9.86	7.20	5.56	5.49	5.12	5.91	4.32	5.27	26.50	27.47	11.57
30	9.87	7.22	5.57	5.49	5.13	5.92	4.33	5.27	26.52	27.50	11.59
40	9.89	7.24	5.58	5.50	5.14	5.93	4.34	5.28	26.56	27.54	11.62
50	9.91	7.24	5.59	5.51	5.14	5.93	[illegible]	5.28	26.58	27.56	11.64
60	9.92	7.26	5.60	5.51	5.14	5.94	4.37	5.29	26.61	27.60	11.66
70	9.95	7.28	5.60	5.52	5.14	5.95	4.38	5.29	26.64	27.62	11.68
80	9.96	7.29	5.61	5.52	5.15	5.95	4.39	5.30	26.67	27.65	11.70
90	9.98	7.30	5.61	5.53	5.15	5.96	4.40	5.30	26.70	27.68	11.72
1300	10.00	7.32	5.62	5.54	5.16	5.98	4.42	5.30	26.71	27.70	11.75
10	10.01	7.33	5.63	5.54	5.16	5.99	4.43	5.31	26.74	27.73	11.77
20	10.02	7.34	5.64	5.55	5.16	5.99	4.44	5.32	26.77	27.76	11.79
30	10.04	7.36	5.64	5.56	5.16	6.00	4.45	5.32	26.80	27.79	11.81
40.	10.06	7.38	5.65	5.56	5.17	6.00	4.46	5.33	26.82	27.82	11.83
50	10.08	7.39	5.65	5.57	5.17	6.01	4.48	5.34	26.85	27.84	11.85
60	10.09	7.40	5.66	5.58	5.18	6.02	4.49	5.34	26.87	27.86	11.87
70	10.11	7.42	5.66	5.58	5.18	6.02	4.50	5.35	26.90	27.89	11.89
80	10.12	7.43	5.67	5.59	5.18	6.03	4.51	5.35	26.92	27.91	11.91
90	10.14	7.45	5.68	5.60	5.19	6.03	4.52	5.36	26.95	27.94	11.93
1400	10.15	7.46	5.68	5.60	5.19	6.03	4.53	5.36	26.97	27.96	11.95
10	10.17	7.48	5.69	5.61	5.20	6.04	4.54	5.37	27.00	27.98	11.97
20	10.18	7.49	5.70	5.61	5.20	[illegible]	[illegible]	5.37	27.02	28.00	12.00
30	10.20	7.50	5.70	5.62	5.20	6.05	4.56	5.38	27.05	28.02	12.02
40	10.22	7.52	5.71	5.62	5.21	6.06	4.58	5.38	27.07	28.04	12.04
50	10.23	7.53	5.72	5.63	5.21	6.06	4.59	5.39	27.09	28.06	12.06
60	10.24	7.54	5.72	5.64	5.21	6.07	4.60	5.40	27.11	28.08	12.08
70	10.26	7.56	5.72	5.64	5.22	6.07	4.60	5.40	27.13	28.10	12.10
80	10.28	7.58	5.73	5.65	5.22	6.08	4.61	5.41	27.16	28.12	12.12
90	10.29	7.59	5.73	5.65	5.22	6.08	4.62	5.41	27.18	28.14	12.14
1500	10.30	7.60	5.74	5.66	[illegible]	6.09	4.63	5.42	27.20	28.16	12.16
10	10.32	7.62	5.75	5.66	[illegible]	6.09	4.64	5.43	27.22	28.18	12.18
20	10.33	7.63	5.75	5.67	[illegible]	6.10	4.65	5.43	27.24	28.20	12.20
30	10.34	7.65	5.76	5.68	[illegible]	6.10	4.66	5.44	27.26	28.22	12.22
40	10.36	7.66	5.76	5.68	5.24	6.11	4.67	5.45	27.28	28.24	12.24
50	10.37	7.68	5.77	5.69	5.25	6.11	4.68	5.45	27.30	28.26	12.26
60	10.38	7.69	5.78	5.69	5.25	6.12	4.69	5.45	27.32	28.27	12.28
70	[illegible]	7.70	5.78	5.70	5.25	6.12	4.70	5.46	27.34	28.29	12.30
80	10.41	7.72	5.79	5.71	5.26	6.13	4.70	5.47	27.36	28.30	12.32
90	10.42	7.73	5.79	5.71	5.27	6.14	4.71	5.48	27.38	28.32	12.34
1600	10.44	7.75	5.80	5.72	5.27	6.14	4.72	5.48	27.40	28.34	12.36
10	10.45	7.76	5.80	5.72	5.28	6.15	4.73	5.49	27.42	28.36	12.38
20	10.46	7.77	5.81	5.73	5.28	6.15	4.74	5.49	27.44	28.37	12.40
30	10.48	7.79	5.81	5.73	5.28	6.16	4.75	5.50	27.46	28.39	12.42
40	10.49	7.80	5.82	5.74	5.29	6.16	4.76	5.50	27.48	28.40	12.44
50	10.50	7.82	5.82	5.74	5.29	6.17	4.76	5.51	27.50	28.42	12.46
60	10.52	7.83	5.83	5.75	5.30	6.17	4.77	5.52	27.52	28.43	12.48
70	10.53	7.84	5.83	5.75	5.30	6.18	4.78	5.52	27.54	28.45	12.50
80	10.54	7.85	5.84	5.76	5.30	6.18	4.78	5.53	27.57	28.47	12.52
90	10.55	7.87	5.84	5.76	5.31	6.19	4.79	5.53	27.57	28.47	12.53

Table 1[illegible] (continued)

Average C_v Over Range from 298 °K to T

(calories/mole/°K)

T, °K	CO_2	H_2O	CO	N_2	H_2	O_2	C(s)	HCl	Al_2O_3	B_2O_3	MgO
1700	10.56	7.88	5.85	5.77	5.31	6.19	4.80	5.54	27.58	28.49	12.55
10	10.58	7.89	5.86	5.77	5.32	6.20	4.81	5.54	27.60	28.50	12.57
20	10.59	7.91	5.86	5.78	5.32	6.20	4.82	5.55	27.62	28.52	12.59
30	10.60	7.92	5.87	5.78	5.33	6.21	4.82	5.55	27.64	28.53	12.61
40	10.61	7.94	5.87	5.79	5.33	6.21	4.83	5.56	27.65	28.54	12.63
50	10.62	7.95	5.88	5.79	5.33	6.22	4.84	5.56	27.67	28.56	12.65
60	10.64	7.96	5.88	5.80	5.34	6.22	4.84	5.57	27.69	28.57	12.67
70	10.65	7.98	5.89	5.80	5.34	6.23	4.85	5.57	27.70	28.58	12.69
80	10.66	7.99	5.89	5.81	5.35	6.23	4.86	5.58	27.72	28.60	12.71
90	10.67	[illegible]	5.90	5.81	5.35	6.24	4.87	5.58	27.73	28.62	12.73
1800	10.68	8.01	5.90	5.82	5.36	6.24	4.88	5.59	27.75	28.63	12.75
10	10.69	8.02	5.90	5.82	5.36	6.24	4.88	5.59	[illegible]	28.64	12.77
20	10.70	8.04	5.91	5.83	5.37	6.25	4.89	5.60	27.78	28.65	12.78
30	10.71	8.05	5.91	5.83	5.37	6.25	4.89	5.60	27.80	28.66	12.80
40	10.72	8.07	5.92	5.83	5.38	6.26	4.90	5.61	27.81	28.68	12.82
50	10.73	8.08	5.92	5.84	5.38	6.26	4.91	5.61	27.82	28.69	12.84
60	10.74	8.09	5.93	5.84	5.38	6.27	4.91	5.62	27.83	28.70	12.86
70	10.76	8.10	5.93	5.85	5.39	6.27	4.92	5.62	27.84	28.71	12.88
80	10.77	8.12	5.94	5.85	5.39	6.28	4.93	5.63	27.86	28.72	12.90
90	10.78	8.13	5.94	5.86	5.40	6.28	4.93	5.64	27.88	28.74	12.92
1900	10.79	8.14	5.94	5.86	5.40	6.29	4.94	5.64	27.89	28.75	12.94
10	10.80	8.16	5.95	5.86	5.41	6.29	4.94	5.65	27.90	28.76	12.96
20	10.81	8.17	5.95	5.87	5.41	6.30	4.95	5.65	27.91	28.77	12.98
30	10.82	8.20	5.96	5.88	5.42	6.30	4.96	5.66	27.92	28.78	13.00
40	10.83	8.20	5.96	5.88	5.42	6.30	4.96	5.66	27.94	28.79	13.02
50	10.84	8.21	5.97	5.88	5.43	6.31	4.97	5.67	27.95	28.80	13.04
60	10.85	8.22	5.97	5.89	5.43	6.31	4.98	5.67	[illegible]	28.81	13.06
70	10.86	8.23	5.98	5.89	5.44	6.32	4.98	5.68	[illegible]	[illegible]	13.08
80	10.87	8.24	5.98	5.90	5.44	6.32	4.99	[illegible]	28.00	28.83	13.10
90	10.88	8.25	5.98	5.90	5.45	6.32	4.99	5.69	28.01	28.84	13.11
2000	10.89	8.26	5.99	5.90	5.45	6.33	5.00	5.70	28.02	28.85	13.13
10	10.90	8.28	5.99	5.91	5.46	6.33	5.01	5.70	28.03	28.86	13.15
20	10.91	8.29	6.00	5.91	5.46	6.34	5.01	5.71	28.04	28.87	13.17
30	10.92	8.30	6.00	5.92	5.47	6.34	5.02	5.71	28.06	28.88	13.18
40	10.93	8.31	6.00	5.92	5.47	6.34	5.02	5.71	28.07	28.89	13.20
50	10.94	8.32	6.01	5.92	5.48	6.35	5.03	5.72	28.08	28.90	13.22
60	10.94	8.33	6.01	5.93	5.48	6.35	5.04	5.72	28.09	28.90	13.24
70	10.95	8.34	6.02	5.93	5.49	6.36	5.04	5.72	28.10	28.91	13.26
80	10.96	8.35	6.02	5.94	5.49	6.36	5.05	5.73	28.12	28.92	13.28
90	10.97	8.36	6.02	5.94	5.50	6.36	5.05	5.73	28.13	28.93	13.29
2100	10.98	8.38	6.03	5.94	5.50	6.37	5.06	5.73	28.14	28.94	13.31
10	10.99	8.39	6.03	5.95	5.50	6.37	5.06	5.74	28.15	28.94	13.33
20	11.00	8.40	6.04	5.95	5.51	6.38	5.07	5.74	28.16	28.95	13.34
30	11.01	8.41	6.04	5.96	5.51	6.38	5.08	5.74	28.17	28.96	13.36
40	11.02	8.42	6.04	5.96	5.52	6.38	5.08	5.75	28.18	28.96	13.38
50	11.02	8.43	6.05	5.96	5.52	6.39	5.09	5.75	28.20	28.97	13.40
60	11.03	8.44	6.05	5.97	5.52	6.39	5.09	5.76	28.21	28.98	13.41
70	11.04	8.45	6.06	5.97	5.53	6.40	5.10	5.76	28.22	28.99	13.42
80	11.05	8.46	6.06	5.97	5.53	6.40	5.10	5.76	28.23	29.00	13.44
90	11.06	8.47	6.06	5.98	5.54	6.40	5.11	5.77	28.24	29.00	13.46
2200	11.06	8.49	6.07	5.98	5.54	6.41	5.11	5.77	28.25	29.01	13.47
10	11.07	8.50	6.07	5.99	5.54	6.41	5.12	5.77	28.26	29.02	13.49
20	11.08	8.51	6.07	5.99	5.55	6.42	5.12	5.78	28.27	29.02	13.50
30	11.09	8.52	6.08	6.00	5.55	6.42	5.13	5.78	28.28	29.03	13.52
40	11.10	8.53	6.08	6.00	5.56	6.42	5.13	5.78	28.29	29.04	13.54
50	11.10	8.54	6.06	6.00	5.56	6.43	5.14	5.79	28.30	29.04	13.56
60	11.11	8.55	6.09	6.01	5.56	6.43	5.14	5.79	28.31	29.05	13.57
70	11.12	8.56	6.09	6.01	5.57	6.44	5.15	5.80	28.32	29.06	13.58
80	11.13	8.57	6.09	6.02	5.57	6.44	5.15	5.80	28.33	29.06	13.60
90	11.14	8.58	6.10	6.02	5.58	6.44	5.16	5.80	28.34	29.07	13.62
2300	11.15	8.59	6.10	6.02	5.58	6.45	5.16	5.81	28.35	29.08	13.63
10	11.15	8.60	6.10	6.03	5.58	6.45	5.17	5.81	28.36	29.08	13.65
20	11.16	8.62	6.11	6.03	5.59	6.46	5.18	5.82	28.37	29.09	13.67
30	11.17	8.63	6.11	6.04	5.59	6.46	5.18	5.82	28.38	29.10	13.68
40	11.18	8.64	6.12	6.04	5.60	6.46	5.19	5.82	28.39	29.10	13.70
50	11.19	8.65	6.12	6.04	5.60	6.46	5.20	5.83	28.40	29.11	13.72
60	11.20	8.66	6.12	6.05	5.60	6.47	5.20	5.83	28.41	29.12	13.73
70	11.20	8.67	6.13	6.05	5.61	6.47	5.20	5.83	28.42	29.12	13.75
80	11.21	8.68	6.13	6.05	5.61	6.48	5.21	5.84	28.43	29.13	13.76
90	11.22	8.69	6.13	6.05	5.62	6.48	5.21	5.84	28.44	29.14	13.78

Table [illegible] (continued)

Average C_v Over Range from 298 °K to T
(calories/mole/°K)

T, °K	CO_2	H_2O	CO	N_2	H_2	O_2	C(s)	HCl	Al_2O_3	B_2O_3	MgO
2400	11.23	8.70	6.14	6.06	5.62	6.48	5.22	5.84	28.45	29.14	13.80
10	11.24	8.71	6.14	6.06	5.63	6.49	5.22	5.85	28.46	29.15	13.82
20	11.24	8.72	6.14	6.06	5.63	6.49	5.23	5.85	28.47	29.15	13.83
30	11.25	8.73	6.15	6.06	5.63	6.49	5.23	5.86	28.48	29.16	13.84
40	11.26	8.74	6.15	6.07	5.64	6.50	5.24	5.86	28.48	29.16	13.86
50	11.27	8.75	6.15	6.07	5.64	6.50	5.24	5.86	28.49	29.17	13.88
60	11.27	8.76	6.16	6.07	5.64	6.50	5.25	5.87	28.50	29.18	13.90
70	11.28	8.77	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
80	11.29	8.78	6.16	6.08	5.65	6.51	5.26	5.88	28.52	29.19	13.93
90	11.30	8.79	6.17	6.08	5.66	6.51	5.26	5.88	28.52	29.19	13.94
2500	11.30	8.79	6.17	6.09	5.66	6.52	5.27	5.88	28.53	29.20	13.96
10	11.31	8.80	6.17	6.09	5.66	6.52	5.27	5.89	28.54	29.20	13.98
20	11.32	8.82	6.17	6.09	5.67	6.52	5.28	5.89	28.55	29.21	14.00
30	11.32	8.83	6.18	6.09	5.67	6.53	5.28	5.90	28.56	29.21	14.02
40	11.33	8.84	6.18	6.10	5.67	6.53	5.28	5.90	28.57	29.22	14.04
50	11.34	8.84	6.18	6.10	5.68	6.54	5.29	5.90	28.58	29.22	14.05
60	11.35	8.85	6.19	6.10	5.68	6.54	5.29	5.90	28.58	29.23	14.07
70	11.36	8.86	6.19	6.10	5.69	6.54	5.30	5.91	28.59	29.23	14.08
80	11.36	8.87	6.19	6.11	5.69	6.54	5.30	5.91	28.60	29.24	14.10
90	11.37	8.88	6.19	6.11	5.69	6.55	5.30	5.91	28.61	29.24	14.12
2600	11.38	8.89	6.20	6.12	5.70	6.55	5.31	5.92	28.62	29.25	14.14
10	11.38	8.90	6.20	6.12	5.70	6.56	5.31	5.92	28.62	29.25	14.16
20	11.39	8.91	6.20	6.12	5.71	6.56	5.32	5.93	28.63	29.26	14.18
30	11.40	8.92	6.21	6.12	5.71	6.56	5.32	5.93	28.64	29.26	14.20
40	11.40	8.93	6.21	6.13	5.72	6.57	5.32	5.93	28.64	29.27	14.21
50	11.41	8.94	6.21	6.13	5.72	6.57	5.33	5.94	28.65	29.27	14.22
60	11.42	8.95	6.21	6.13	5.72	6.57	5.33	5.94	28.66	29.28	14.24
70	11.42	8.96	6.22	6.14	5.73	6.58	5.34	5.94	28.67	29.28	14.26
80	11.43	8.97	6.22	6.14	5.73	6.58	5.34	5.95	28.68	29.29	14.27
90	11.44	8.98	6.22	6.14	5.74	6.58	5.34	5.95	28.68	29.29	14.29
2700	11.44	8.98	6.22	6.14	5.74	6.59	5.35	5.95	28.69	29.30	14.30
10	11.45	8.99	6.23	6.14	5.74	6.59	5.35	5.96	28.70	29.30	14.32
20	11.46	9.00	6.23	6.15	5.75	6.60	5.36	5.96	28.71	29.31	14.34
30	11.46	9.01	6.23	6.15	5.75	6.60	5.36	5.96	28.71	29.31	14.35
40	11.46	9.02	6.23	6.15	5.75	6.60	5.36	5.97	28.72	29.32	14.36
50	11.47	9.03	6.24	6.15	5.76	6.61	5.37	5.97	28.73	29.32	14.38
60	11.48	9.04	6.24	6.16	5.76	6.61	5.37	5.98	28.73	29.33	14.40
70	11.48	9.05	6.24	6.16	5.76	6.61	5.38	5.98	28.74	29.33	14.41
80	11.49	9.06	6.24	6.16	5.77	6.62	5.38	5.98	28.75	29.34	14.42
90	11.50	9.07	6.25	6.17	5.77	6.62	5.38	5.99	28.76	29.34	14.44
2800	11.50	9.08	6.25	6.17	5.77	6.62	5.39	5.99	28.76	29.35	14.45
10	11.51	9.09	6.25	6.17	5.78	6.63	5.39	6.00	28.77	29.35	14.47
20	11.51	9.10	6.25	6.17	5.78	6.63	5.40	6.00	28.77	29.35	14.48
30	11.52	9.11	6.26	6.18	5.79	6.63	5.40	6.00	28.78	29.36	14.50
40	11.53	9.11	6.26	6.18	5.79	6.64	5.40	6.01	28.79	29.36	14.51
50	11.53	9.12	6.26	6.19	5.79	6.64	5.41	6.01	28.80	29.37	14.52
60	11.54	9.13	6.26	6.18	5.80	6.64	5.41	6.02	28.80	29.37	14.54
70	11.54	9.14	6.26	6.19	5.80	6.65	5.41	6.02	28.81	29.38	14.55
80	11.54	9.15	6.27	6.19	5.80	6.65	5.42	6.02	28.82	29.38	14.56
90	11.55	9.16	6.27	6.19	5.81	6.65	5.42	6.03	28.82	29.38	14.58
2900	11.56	9.17	6.27	6.19	5.81	6.66	5.42	6.03	28.83	29.39	14.59
10	11.56	9.17	6.27	6.20	5.81	6.66	5.43	6.03	28.84	29.39	14.60
20	11.56	9.18	6.28	6.20	5.82	6.66	5.43	6.04	28.84	29.40	14.62
30	11.57	9.19	6.28	6.20	5.82	6.66	5.44	6.04	28.85	29.40	14.63
40	11.57	9.20	6.28	6.20	5.83	6.67	5.44	6.04	28.85	29.40	14.64
50	11.57	9.21	6.28	6.21	5.83	6.67	5.44	6.05	28.86	29.41	14.65
60	11.57	9.22	6.29	6.21	5.83	6.67	5.45	6.05	28.86	29.41	14.67
70	11.58	9.23	6.29	6.21	5.84	6.68	5.46	6.06	28.87	29.42	14.68
80	11.59	9.23	6.29	6.21	5.84	6.68	5.45	6.06	28.88	29.42	14.69
90	11.59	9.24	6.29	6.22	5.84	6.68	5.46	6.06	28.89	29.42	14.70
3000	11.60	9.25	6.29	6.22	5.85	6.69	5.46	6.07	28.90	29.43	14.71
10	11.61	9.26	6.30	6.22	5.85	6.69	5.46	6.07	28.90	29.43	14.73
20	11.62	[illegible]	6.30	6.22	5.86	6.69	5.47	6.07	28.91	29.44	14.74
30	11.62	[illegible]	6.30	6.23	5.86	6.70	5.47	6.08	28.92	29.44	14.75
40	11.62	[illegible]	6.30	6.23	5.86	6.70	5.47	6.08	28.92	29.44	14.76
50	11.63	9.29	6.30	6.23	5.87	6.70	5.48	6.08	28.93	29.45	14.78
60	11.64	9.30	6.31	6.23	5.87	6.71	5.48	6.09	28.94	29.45	14.79
70	11.64	9.30	6.31	6.23	5.87	6.71	5.48	6.09	28.94	29.45	14.80
80	11.65	9.31	6.31	6.24	5.88	6.71	5.49	6.10	28.95	29.46	[illegible]
90	11.65	9.31	6.31	6.24	5.88	6.72	5.49	6.10	28.95	29.46	14.82

Table 1[illegible] (continued)

Average C_v Over Range from 298 °K to T

(calories/mole/°K)

T, °K	CO_2	H_2O	CO	N_2	H_2	O_2	C(s)	HCl	Al_2O_3	B_2O_3	MgO
3100	11.66	9.32	6.32	6.24	5.88	6.72	5.49	6.10	28.96	29.46	14.83
10	11.66	9.33	6.32	6.24	5.89	6.72	5.50	6.11	28.96	29.47	14.84
20	11.66	9.34	6.32	6.24	5.89	6.73	5.50	6.11	28.97	29.47	14.86
30	11.67	9.34	6.32	6.25	5.89	6.73	5.50	6.11	28.98	29.48	14.87
40	11.68	9.35	6.32	6.25	5.90	6.73	5.51	6.12	28.98	29.48	14.88
50	11.68	9.36	6.32	6.25	5.90	6.74	5.51	6.12	28.99	29.48	14.89
60	11.69	9.37	6.33	6.25	5.90	6.74	5.52	6.12	29.00	29.49	14.90
70	11.69	9.38	6.33	6.26	5.91	6.74	5.52	6.13	29.00	29.49	14.91
80	11.70	9.38	6.33	6.26	5.91	6.74	5.52	6.13	[illegible]	[illegible]	[illegible]
90	11.70	9.39	6.33	6.26	5.91	6.75	5.52	6.14	29.01	29.50	14.93
3200	11.71	9.40	6.34	6.26	5.92	6.75	5.53	6.14	29.02	29.50	14.94
10	11.72	9.41	6.34	6.26	5.92	6.75	5.53	6.14	29.02	29.50	14.95
20	11.72	9.41	6.34	6.26	5.92	6.76	5.54	6.15	29.03	29.51	14.96
30	11.72	9.42	6.34	6.27	5.93	6.76	5.54	6.15	29.03	29.51	14.97
40	11.73	9.42	6.34	6.27	5.93	6.76	5.54	6.16	29.04	29.51	14.98
50	11.73	9.43	6.34	6.27	5.94	6.76	5.54	6.16	29.04	29.52	14.99
60	11.74	9.44	6.35	6.28	5.94	6.77	5.55	6.16	29.05	29.52	15.00
70	11.74	9.44	6.35	6.28	5.94	6.77	5.55	6.16	29.05	29.52	15.01
80	11.75	9.45	6.35	6.28	5.94	6.77	5.55	6.17	29.06	29.53	15.02
90	11.75	9.46	6.35	6.28	5.95	6.78	5.56	6.17	29.06	29.53	15.03
3300	11.76	9.47	6.36	6.28	5.95	6.78	5.56	6.18	29.07	29.53	15.04
10	11.76	9.48	6.36	6.29	5.96	6.79	5.56	6.18	29.07	29.54	15.05
20	11.77	9.48	6.36	6.29	5.96	6.78	5.56	6.18	29.08	29.54	15.06
30	11.77	9.49	6.36	6.29	5.96	6.79	5.57	6.19	29.08	[illegible]	[illegible]
40	11.78	9.49	6.36	6.29	5.96	6.79	5.57	6.19	29.09	29.54	15.08
50	11.78	9.50	6.36	6.29	5.97	6.80	5.57	6.20	29.09	29.55	15.09
60	11.79	9.51	6.37	6.30	5.97	6.80	5.58	6.20	29.10	29.55	15.10
70	11.80	9.52	6.37	6.30	5.98	6.80	5.58	6.20	29.10	29.55	15.11
80	11.80	9.52	6.37	6.30	5.98	6.80	5.58	6.21	29.11	29.56	15.12
90	11.80	9.53	6.37	6.30	5.98	6.81	5.59	6.21	29.11	29.56	15.13
3400	11.81	9.53	6.37	6.30	5.98	6.81	5.59	6.22	29.12	29.56	15.14
10	11.82	9.54	6.38	6.31	5.99	6.81	5.59	6.22	29.12	29.56	15.15
20	11.82	9.54	6.38	6.31	5.99	6.82	5.60	6.22	29.13	29.57	15.16
30	11.82	9.55	6.38	6.31	5.99	6.82	5.60	[illegible]	[illegible]	29.57	15.17
40	11.83	9.56	6.38	6.31	6.00	6.82	5.60	6.23	29.14	29.57	15.18
50	11.83	9.56	6.38	6.32	6.00	6.82	5.61	6.24	29.14	29.58	15.19
60	11.84	9.57	6.39	6.32	6.01	6.83	5.61	6.24	29.14	29.58	15.20
70	11.84	9.58	6.39	6.32	6.01	6.83	5.61	6.24	29.15	29.58	15.21
80	11.84	9.58	6.39	6.32	6.01	6.83	5.62	6.24	29.15	29.58	15.22
90	11.85	9.59	6.39	6.32	6.02	6.84	5.62	6.25	29.16	29.59	15.23
3500	11.85	9.60	6.39	6.32	6.02	6.84	5.62	6.25	29.16	29.59	15.24
10	11.86	9.60	6.39	6.33	6.02	6.84	5.62	6.26	29.16	29.59	15.25
20	11.86	9.61	6.40	6.33	[illegible]	6.84	5.63	6.26	29.17	29.60	15.26
30	11.86	9.62	6.40	6.33	6.03	6.85	5.63	6.26	29.17	29.60	15.27
40	11.87	9.62	6.40	6.33	6.03	6.85	5.63	6.27	29.18	29.60	15.28
50	11.87	9.63	6.40	6.34	6.03	6.85	5.64	6.27	29.18	29.60	15.28
60	11.88	9.64	6.40	6.34	[illegible]	6.86	5.64	6.28	29.19	29.60	15.29
70	11.88	9.64	6.40	6.34	6.04	6.86	5.64	6.28	29.19	29.60	15.30
80	11.88	9.65	6.41	6.34	6.04	6.86	5.64	6.28	29.20	29.61	15.32
90	11.89	9.66	6.41	6.34	6.05	6.36	5.65	6.29	29.20	29.61	15.32
3600	11.59	9.66	6.41	6.35	6.05	6.87	5.65	6.29	29.20	29.61	15.33
10	11.90	9.67	6.41	6.35	6.05	6.87	5.65	6.30	29.21	29.62	15.34
20	11.90	9.68	6.42	6.35	6.06	6.87	5.66	6.30	29.21	29.62	15.35
30	11.90	9.68	6.42	6.35	6.06	6.88	5.66	6.30	29.22	29.62	15.36
40	11.91	9.69	6.42	6.36	6.06	6.88	5.66	6.31	29.22	29.62	15.36
50	11.91	9.70	6.42	6.36	6.06	6.88	5.66	6.31	29.22	29.63	15.37
60	11.91	9.70	6.42	6.36	6.07	6.88	5.67	6.31	29.23	29.62	15.38
70	11.92	9.71	6.42	6.36	6.07	6.89	5.67	6.32	29.23	29.63	15.39
80	11.92	9.72	6.42	6.36	6.07	6.89	5.67	6.32	29.24	29.63	15.40
90	11.93	9.72	6.42	6.36	6.08	6.89	5.68	6.33	29.24	29.64	15.41
3700	11.93	9.73	6.43	6.37	6.08	6.89	5.68	6.33	29.24	29.64	15.42
10	11.94	9.73	6.43	6.37	6.08	6.90	5.68	6.33	29.25	29.64	15.42
20	11.94	9.74	6.43	6.37	6.09	6.90	5.69	6.34	29.25	29.64	15.43
30	11.94	9.74	6.43	6.37	6.09	6.90	5.69	6.34	29.26	29.65	15.44
40	11.95	9.75	6.44	6.37	6.09	6.90	5.69	6.34	29.26	29.65	15.45
50	11.95	9.76	6.44	6.38	6.10	6.91	5.70	6.35	29.26	29.65	15.46
60	11.96	9.76	6.44	6.38	6.10	6.91	5.70	6.35	29.27	29.66	15.46
70	11.96	9.77	6.44	6.38	6.10	[illegible]	5.70	6.36	29.27	29.66	15.47
80	11.97	9.77	6.44	6.38	6.10	6.92	[illegible]	6.36	29.28	29.66	15.48
90	11.97	9.78	6.44	6.38	6.11	[illegible]	5.71	6.36	29.28	29.66	15.49

Table ... (continued)

Average C_v Over Range from 298 to T

(calories/mole/°K)

T, °K	CO_2	H_2O	CO	N_2	H_2	O_2	C(s)	HCl	Al_2O_3	B_2O_3	MgO
3800	11.98	9.78	6.45	6.38	6.11	6.92	5.71	6.37	29.28	29.66	15.50
10	11.98	9.79	6.45	6.38	6.11	6.93	5.71	6.37	29.29	29.67	15.51
20	11.98	9.80	6.45	6.39	6.12	6.93	5.72	6.38	29.29	29.67	15.52
30	11.99	9.80	6.45	6.39	6.12	6.93	5.72	6.38	29.30	29.67	15.52
40	11.99	9.81	6.45	6.39	6.12	6.93	5.72	6.30	29.30	29.68	15.53
50	12.00	9.82	6.45	6.39	6.12	6.94	5.72	6.39	29.30	29.68	15.54
60	12.00	9.82	6.46	6.39	6.13	6.94	5.73	6.39	29.31	29.68	15.55
70	12.00	9.83	6.46	6.40	6.13	6.94	5.73	6.40	29.31	29.68	15.56
80	12.01	9.83	6.46	6.40	6.14	6.94	5.73	6.40	29.32	29.68	15.56
90	12.01	9.84	[illegible]	[illegible]	6.14	6.94	5.74	[illegible]	29.32	[illegible]	[illegible]
3900	12.02	9.84	6.46	6.40	6.14	6.95	5.74	6.41	29.32	29.69	15.58
10	12.02	9.85	6.46	6.40	6.14	6.95	5.74	6.41	29.32	29.69	15.59
20	12.02	9.86	6.46	6.41	6.15	6.95	5.75	6.41	29.33	29.69	15.60
30	12.03	9.86	6.47	6.41	6.15	6.96	5.75	6.42	29.33	29.69	15.61
40	12.03	9.87	6.47	6.41	6.15	6.96	5.75	6.42	29.33	29.70	15.62
50	12.03	9.88	6.47	6.41	6.16	6.96	5.76	6.42	29.34	29.70	15.62
60	12.04	9.88	6.47	6.41	6.16	6.96	5.76	6.43	29.34	29.70	15.63
70	12.04	9.89	6.47	6.42	6.16	6.97	5.76	6.43	29.34	29.70	15.64
80	12.04	9.89	6.47	6.42	6.16	6.97	5.76	6.44	29.34	29.70	15.64
90	12.04	9.90	6.48	6.42	6.17	6.97	5.77	6.44	29.35	29.71	15.65
4000	12.05	9.90	6.48	6.42	6.17	6.98	5.77	6.45	29.35	29.71	15.66
10	12.05	9.91	6.48	6.42	6.17	6.99	5.77	6.45	29.35	29.71	15.66
20	12.06	9.92	6.48	6.42	6.17	6.98	5.78	6.45	29.36	29.72	15.67
30	12.06	9.92	6.48	6.42	6.18	6.98	5.78	6.46	29.36	29.72	15.68
40	12.06	9.93	6.48	6.42	6.18	6.98	5.78	6.46	29.37	29.72	15.69
50	12.06	9.93	6.48	6.42	6.18	6.99	5.78	6.46	29.37	29.72	15.70
60	12.07	9.94	6.48	6.43	6.18	6.99	5.79	6.46	29.38	29.72	15.70
70	12.07	9.94	6.48	6.43	6.18	6.99	5.79	6.47	29.38	29.72	15.71
80	12.07	9.95	6.49	6.43	6.19	6.99	5.79	6.47	29.38	29.73	15.72
90	12.08	9.95	6.49	6.43	6.19	7.00	5.80	6.47	29.39	29.73	15.74
4100	12.08	9.96	6.49	6.43	6.19	7.00	5.80	6.48	29.39	29.73	15.73
10	12.08	9.96	6.49	6.44	6.20	7.00	5.80	6.48	29.39	29.73	15.74
20	12.08	9.97	6.49	6.44	6.20	7.00	5.80	6.49	29.40	29.74	15.74
30	12.09	9.97	6.49	6.44	6.20	7.01	5.81	6.49	29.40	29.74	15.75
40	12.10	9.98	6.50	6.44	6.20	7.01	5.81	6.50	29.40	29.74	15.76
50	12.10	9.98	6.50	6.44	6.21	7.01	5.81	6.50	29.41	29.74	15.76
60	12.10	9.99	6.50	6.44	6.21	7.02	5.82	6.50	29.41	29.74	15.77
70	12.11	9.99	6.50	6.45	6.21	7.02	5.82	6.51	29.42	29.75	15.78
80	12.12	10.00	6.50	6.45	6.21	7.02	5.82	6.51	29.42	29.75	15.78
90	12.12	10.00	6.50	6.45	6.22	7.02	5.82	6.52	29.42	29.75	15.79
4200	12.12	10.01	6.50	6.45	6.22	7.02	5.83	6.52	29.43	29.75	15.79
10	12.12	10.02	6.50	6.45	6.22	7.03	5.83	6.52	29.43	29.76	15.80
20	12.12	10.02	6.51	6.45	6.22	7.03	5.83	6.53	29.43	29.76	15.80
30	12.12	10.03	6.51	6.46	6.23	7.03	5.84	6.53	29.44	29.76	15.81
40	12.13	10.03	6.51	6.46	6.23	7.04	5.84	6.53	29.44	29.76	15.82
50	12.13	10.04	6.51	6.46	6.23	7.04	5.84	6.54	29.44	29.76	15.82
60	12.13	10.04	6.51	6.46	6.24	7.04	5.84	6.54	29.45	29.76	15.83
70	12.14	10.05	6.51	6.46	6.24	7.04	5.85	6.54	29.45	29.77	15.84
80	12.14	10.05	6.51	6.46	6.24	7.05	5.85	6.55	29.46	29.77	15.84
90	12.14	10.06	6.51	6.47	6.24	7.05	5.85	6.55	29.46	29.77	15.85
4300	12.14	10.06	6.52	6.47	6.25	7.05	5.86	6.56	29.46	29.77	15.86
10	12.15	10.07	6.52	6.47	6.25	7.05	5.86	6.56	29.46	29.78	15.86
20	12.15	10.07	6.52	6.47	6.25	7.06	5.86	6.56	29.47	29.78	15.87
30	12.16	10.08	6.52	6.47	6.25	7.06	5.87	6.57	29.47	29.78	15.87
40	12.16	10.08	6.52	6.47	6.26	7.06	5.87	6.57	29.47	29.78	15.88
50	[illegible]	[illegible]	[illegible]	6.48	6.26	7.06	5.87	6.58	29.48	29.78	15.88
60	12.17	10.09	6.52	6.48	6.26	7.07	5.88	6.58	29.48	29.78	15.89
70	12.17	10.10	6.52	6.48	6.26	7.07	5.88	6.58	29.48	29.78	15.89
80	12.17	10.10	6.52	6.48	6.27	7.07	5.88	6.59	29.48	29.79	15.90
90	12.18	10.11	6.53	6.48	6.27	7.07	5.88	6.59	29.49	29.79	15.90
4400	12.18	10.11	6.53	6.48	6.27	7.08	5.89	6.59	29.49	29.79	15.91
10	12.18	10.12	6.53	6.48	6.27	7.08	5.89	6.60	29.49	29.79	15.92
20	12.19	10.12	6.53	6.49	6.27	7.08	5.89	6.60	29.50	29.79	15.92
30	12.19	10.13	6.53	6.49	6.28	7.08	5.90	6.60	29.50	29.80	15.92
40	12.20	10.14	6.53	6.49	6.28	7.08	5.90	6.61	29.50	29.80	15.93
50	12.20	10.14	6.53	6.49	6.28	7.09	5.90	6.61	29.51	29.80	15.94
60	12.20	10.15	6.54	6.49	6.28	7.09	5.91	6.62	29.51	29.80	15.94
70	12.21	10.15	6.54	6.49	6.29	7.09	5.91	6.62	29.51	29.80	15.95
80	12.21	10.16	6.54	6.49	6.29	7.09	5.91	6.62	29.52	29.80	15.95
90	12.21	10.16	6.54	6.50	6.29	7.10	5.92	6.63	29.52	29.80	15.96

Table [illegible] (continued)

Average C_v Over Range from 298 °K to T
(calories/mole/°K)

T, °K	CO_2	H_2O	CO	N_2	H_2	O_2	C(s)	HCl	Al_2O_3	B_2O_3	MgO
4500	12.22	10.17	6.54	6.50	6.30	7.10	5.92	6.63	29.52	29.80	15.96
10	12.22	10.17	6.54	6.50	6.30	7.10	5.92	6.64	29.52	29.80	15.97
20	12.22	10.18	6.54	6.50	6.30	7.10	5.93	6.64	29.53	29.81	15.97
30	12.23	10.18	6.54	6.50	6.30	7.10	5.93	6.64	29.53	29.81	15.98
40	12.23	10.19	6.54	6.50	6.30	7.10	5.93	6.65	29.53	29.82	15.98
50	12.23	10.19	6.55	6.50	6.31	7.11	5.94	6.65	29.54	29.82	15.99
60	12.23	10.20	6.55	6.51	6.31	7.11	5.94	6.66	29.54	29.81	15.99
70	12.24	10.20	6.55	6.51	6.31	7.11	5.94	6.66	29.54	29.81	16.00
80	12.24	10.20	6.55	6.51	6.31	7.12	5.94	6.66	29.54	29.82	16.00
90	12.24	10.21	6.55	6.51	6.32	7.12	5.95	6.67	29.55	29.82	16.01
4600	12.25	10.21	6.55	6.51	6.32	7.12	5.95	6.67	29.55	29.82	16.01
10	12.25	10.22	6.55	6.51	6.32	7.12	5.95	6.68	29.55	29.82	16.02
20	12.25	10.22	6.55	6.51	6.32	7.12	5.96	6.68	29.55	29.82	16.02
30	12.26	10.23	6.56	6.52	6.33	7.12	5.96	6.68	29.56	29.82	16.03
40	12.26	10.23	6.56	6.52	6.33	7.13	5.96	6.68	29.56	29.82	16.03
50	12.26	10.24	6.56	6.52	6.33	7.13	5.96	6.69	29.56	29.82	16.04
60	12.27	10.24	6.56	6.52	6.33	7.13	5.97	6.69	29.56	29.82	16.04
70	12.27	10.25	6.56	6.52	6.34	7.14	5.97	6.70	29.56	29.83	16.05
80	12.27	10.25	6.56	6.52	6.34	7.14	5.97	6.70	29.57	29.83	16.05
90	12.27	10.26	6.56	6.52	6.34	7.14	5.97	6.70	29.57	29.83	16.06
4700	12.28	10.26	6.56	6.52	6.34	7.14	5.98	6.71	29.57	29.83	16.06
10	12.28	10.26	6.56	6.53	6.34	7.14	5.98	6.71	29.58	29.83	16.06
20	12.28	10.27	6.56	6.53	6.35	7.14	5.98	6.72	29.58	29.84	16.07
30	12.28	10.27	6.57	6.53	6.35	7.15	5.99	6.72	29.58	29.84	16.07
40	12.29	10.28	6.57	6.53	6.35	7.15	5.99	6.72	29.58	29.84	16.08
50	12.29	10.28	6.57	6.53	6.35	7.15	5.99	6.72	29.59	29.84	16.08
60	12.29	10.29	6.57	6.53	6.36	7.15	5.99	6.73	29.59	29.84	16.09
70	12.30	10.29	6.57	6.53	6.36	7.16	6.00	6.74	29.59	29.84	16.09
80	12.30	10.30	6.57	6.54	6.36	7.16	6.00	6.74	29.59	29.84	16.10
90	12.30	10.30	6.57	6.54	6.36	7.16	6.00	6.74	29.60	29.84	16.10
4800	12.31	10.31	6.57	6.54	6.36	7.16	6.00	6.75	29.60	29.84	16.10
10	12.31	10.31	6.57	6.54	6.37	7.16	6.01	6.75	29.60	29.84	16.11
20	12.32	10.31	6.58	6.54	6.37	7.17	6.01	6.75	29.60	29.84	16.11
30	12.32	10.32	6.58	6.54	6.37	7.17	6.01	6.76	29.60	29.85	16.12
40	12.32	10.32	6.58	6.54	6.37	7.17	6.02	6.76	29.61	29.85	16.12
50	12.32	10.33	6.58	6.55	6.37	7.17	6.02	6.76	29.61	29.85	16.13
60	12.32	10.33	6.58	6.55	6.38	7.17	6.02	6.77	29.61	29.85	16.13
70	12.32	10.34	6.58	6.55	6.38	7.18	6.03	6.77	29.61	29.85	16.14
80	12.33	10.34	6.58	6.55	6.38	7.16	6.03	6.78	29.62	29.85	16.14
90	12.33	10.34	6.58	6.55	6.38	7.18	6.03	6.78	29.62	29.85	16.14
4900	12.33	10.35	6.58	6.55	6.38	7.18	6.04	6.78	29.62	29.85	16.15
10	12.34	10.35	6.58	6.55	6.38	7.18	6.04	6.79	29.62	29.86	16.15
20	12.34	10.36	6.59	6.55	6.39	7.19	6.04	6.79	29.63	29.86	16.16
30	12.34	10.36	6.59	6.56	6.39	7.19	6.04	6.80	29.63	29.86	16.16
40	12.34	10.36	6.59	6.56	6.39	7.19	6.05	6.80	29.63	29.86	16.16
50	12.35	10.37	6.59	6.56	6.39	7.19	6.05	6.80	29.64	29.86	16.17
60	12.35	10.37	6.59	6.56	6.39	7.20	6.05	6.81	29.64	29.86	16.17
70	12.36	10.38	6.59	6.56	6.40	7.20	6.06	6.81	29.64	29.86	16.18
80	12.36	10.38	6.59	6.56	6.40	7.20	6.06	6.82	29.64	29.86	16.18
90	12.36	10.38	6.59	6.56	6.40	7.20	6.06	6.82	29.64	29.86	16.18
5000	12.36	10.39	6.59	6.56	6.40	7.20	6.06	6.82	29.64	29.86	16.18
10	12.36	10.40	6.60	6.56	6.40	7.21	6.07	6.83	29.64	29.85	16.19
20	12.37	10.40	6.60	6.56	6.41	7.21	6.07	6.83	29.64	29.86	16.19
30	12.37	10.40	6.60	6.57	6.41	7.21	6.08	6.84	29.65	29.86	16.20
40	12.38	10.41	6.60	6.57	6.41	7.22	6.08	6.84	29.65	29.86	16.20
50	12.38	10.41	6.60	6.57	6.41	7.22	6.08	6.84	29.65	29.86	16.20
60	12.38	10.42	6.60	6.57	6.41	7.22	6.09	6.85	29.66	29.86	16.21
70	12.38	10.42	6.60	6.57	6.42	7.22	6.09	6.85	29.66	29.87	16.21
80	12.39	10.42	6.60	6.57	6.43	7.22	6.09	6.86	29.66	29.87	16.22
90	12.39	[illegible]	6.60	6.57	6.42	7.22	6.09	6.86	29.66	29.87	16.22
5100	12.39	10.43	6.61	6.57	[illegible]	7.22	6.10	6.86	29.66	29.87	16.22
10	12.40	10.44	6.61	6.58	6.42	7.22	6.10	6.87	29.67	29.87	16.23
20	12.40	10.44	6.61	6.58	6.43	7.23	6.10	6.87	29.67	29.87	16.23
30	12.40	10.45	6.61	6.58	6.43	7.23	6.10	6.87	29.67	29.87	16.24
40	12.40	10.45	6.61	6.58	6.43	7.23	6.11	6.88	29.67	29.88	16.24
50	12.41	10.46	6.61	6.58	6.43	7.23	6.11	6.88	29.68	29.88	16.24
60	12.41	10.46	6.61	6.58	6.44	7.24	6.11	6.88	29.68	29.88	16.25
70	12.41	10.46	6.61	6.58	6.44	7.24	6.12	6.89	29.68	29.88	16.25
80	12.42	10.47	6.61	6.58	6.44	7.24	6.12	6.89	29.68	29.88	16.25
90	12.42	10.47	6.62	6.59	6.44	7.24	6.12	6.90	29.68	29.88	16.26

Table 149 (continued)

Average C_v Over Range from 298 °K to T
(calories/mole/°K)

T, °K	CO_2	H_2O	CO	N_2	H_2	O_2	C(s)	HCl	Al_2O_3	B_2O_3	MgO
5200	12.42	10.48	6.62	6.59	6.44	7.25	6.13	6.90	29.68	29.88	16.26
10	12.42	10.48	6.62	6.59	6.45	7.25	6.13	6.90	29.68	29.88	16.27
20	12.43	10.49	6.62	6.59	6.45	7.25	6.13	6.91	29.69	29.88	16.27
30	12.43	10.49	6.62	6.59	6.45	7.25	6.14	6.91	29.69	29.88	16.28
40	12.44	10.49	6.62	6.59	6.45	7.26	6.14	6.92	29.69	29.88	16.28
50	12.44	10.50	6.62	6.59	6.45	7.26	6.14	6.92	29.69	29.88	16.28
60	12.44	10.50	6.62	6.59	6.45	7.26	6.14	6.92	29.69	29.88	16.28
70	12.44	10.51	6.62	6.59	6.46	7.26	6.15	6.93	29.70	29.88	16.29
80	12.45	10.51	6.62	6.60	6.46	7.26	6.15	6.93	29.70	29.88	16.29
90	12.45	10.52	6.63	[illegible]	6.46	7.27	6.15	6.94	29.70	29.88	16.30
5300	12.45	10.52	6.63	6.60	6.46	7.27	6.16	6.94	29.70	29.88	16.30
10	12.46	10.53	6.63	6.60	6.46	7.27	6.16	6.94	29.70	29.89	16.30
20	12.46	10.53	6.63	6.60	6.47	7.28	6.16	6.94	29.71	29.89	16.31
30	12.46	10.54	6.63	6.60	6.47	7.28	6.16	6.95	29.71	29.89	16.31
40	12.46	10.54	6.63	6.60	6.47	7.28	6.16	6.95	29.71	29.89	16.32
50	12.47	10.54	6.63	6.60	6.47	7.28	6.17	6.96	29.71	29.89	16.32
60	12.47	10.55	6.63	6.61	6.47	7.28	6.17	6.96	29.71	29.89	16.32
70	12.47	10.55	6.63	6.61	6.48	7.28	6.18	6.96	29.72	29.89	16.33
80	12.48	10.56	6.64	6.61	6.48	7.29	6.18	6.97	29.72	29.89	16.33
90	12.48	10.56	6.64	6.61	6.48	7.29	6.19	6.97	29.72	29.90	16.33
5400	12.48	10.56	6.64	6.61	6.48	7.29	6.19	6.97	29.72	29.90	16.34
10	12.48	10.57	6.64	6.61	6.48	7.29	6.19	6.98	29.72	29.90	16.34
20	12.49	10.57	6.64	6.61	6.49	7.29	6.20	6.98	29.72	29.90	16.34
30	12.49	10.58	6.64	6.61	6.49	7.29	6.20	6.98	29.73	29.90	16.35
40	12.49	10.58	6.64	6.62	6.49	7.30	6.20	6.99	29.73	29.90	16.35
50	12.50	10.59	6.64	6.62	6.49	7.30	6.20	6.99	29.73	29.90	16.36
60	12.50	10.59	6.64	6.62	6.49	7.30	6.21	7.00	29.73	29.90	16.36
70	12.50	10.59	6.64	6.62	6.50	7.30	6.21	7.00	29.74	29.90	16.36
80	12.50	10.60	6.64	6.62	6.50	7.30	6.21	7.00	29.74	29.90	16.37
90	12.51	10.60	6.65	6.62	6.50	7.31	6.22	7.01	29.74	29.90	16.37
5500	12.51	10.61	6.65	6.62	6.50	7.31	6.22	7.01	29.74	29.90	16.37
10	12.51	10.61	6.65	6.62	6.50	7.31	6.22	7.02	29.74	29.91	16.38
20	12.52	10.62	6.65	6.63	6.51	7.31	6.23	7.02	29.74	29.91	16.38
30	12.52	10.62	6.65	6.63	6.51	7.32	6.23	7.02	29.75	29.91	16.38
40	12.52	10.62	6.65	6.63	6.51	7.32	6.23	7.03	29.75	29.91	16.39
50	12.52	10.63	6.65	6.63	6.51	7.32	6.24	7.03	29.75	29.91	16.39
60	12.53	10.63	6.65	6.63	6.51	7.32	6.24	7.04	29.75	29.91	16.40
70	12.53	10.64	6.65	6.63	6.52	7.32	6.24	7.04	29.76	29.91	16.40
80	12.53	10.64	6.66	6.63	6.52	7.33	6.24	7.04	29.76	29.91	16.40
90	12.54	10.65	6.66	6.63	6.52	7.33	6.25	7.04	29.76	29.91	16.41
5600	12.54	10.65	6.66	6.63	6.52	7.33	6.25	7.05	29.76	29.92	16.41
10	12.54	10.66	6.66	6.63	6.53	7.33	6.25	7.05	29.76	29.92	16.42
20	12.54	10.66	6.66	6.64	6.53	7.33	6.25	7.06	29.76	29.92	16.42
30	12.55	10.66	6.66	6.64	6.53	7.34	6.26	7.06	29.76	29.92	16.42
40	12.55	10.67	6.66	6.64	6.53	7.34	6.26	7.06	29.77	29.92	16.42
50	12.55	10.67	6.66	6.64	6.53	7.34	6.27	7.07	29.77	29.92	16.43
60	12.56	10.68	6.66	6.64	6.54	7.34	6.27	7.07	29.77	29.92	16.43
70	12.56	10.68	6.66	6.64	6.54	7.34	6.27	7.06	29.77	29.92	16.44
80	12.56	10.69	6.67	6.64	6.54	7.35	6.28	7.08	29.78	29.92	16.44
90	12.56	10.69	6.67	6.64	6.54	7.35	6.28	7.08	29.78	29.92	16.44
5700	12.57	10.69	6.67	6.65	6.54	7.35	6.28	7.09	29.78	29.92	16.45
10	12.57	10.70	6.67	6.65	6.55	7.35	6.28	7.09	29.78	29.92	16.45
20	12.57	10.70	6.67	6.65	6.55	7.35	6.29	7.10	29.78	29.92	16.46
30	12.58	10.71	6.67	6.65	6.55	7.35	6.29	7.10	29.78	29.93	16.46
40	12.58	10.71	6.67	6.65	6.55	7.36	6.30	7.10	29.78	29.93	16.46
50	12.58	10.72	6.67	6.65	6.55	7.36	6.30	7.11	29.79	29.93	16.46
60	12.59	10.72	6.67	6.65	6.56	7.36	6.30	7.11	29.79	29.93	16.47
70	12.59	10.72	6.68	6.65	6.55	7.36	6.30	7.12	29.79	29.93	16.47
80	12.59	10.73	6.68	6.66	6.56	7.36	6.31	7.12	29.80	29.93	16.48
90	12.60	10.73	6.68	6.66	6.56	7.36	6.31	7.12	29.80	29.93	16.48
5800	12.60	10.74	6.68	6.66	6.56	7.37	6.31	7.12	29.80	29.93	16.48
10	12.60	10.75	6.68	6.66	6.57	7.37	6.31	7.13	29.80	29.93	16.48
20	12.60	10.75	6.68	6.66	6.57	7.37	6.32	7.13	29.80	29.93	16.47
30	12.61	10.75	6.68	6.66	6.57	7.38	6.32	7.14	29.80	29.93	16.49
40	12.61	10.76	6.68	6.67	6.57	7.38	6.32	7.14	29.81	29.93	16.50
50	12.62	10.76	6.69	6.67	6.57	7.38	6.33	7.14	29.81	29.94	16.50
60	12.62	10.76	6.69	6.67	6.58	7.38	6.33	7.15	29.81	29.94	16.50
70	12.62	10.77	6.69	6.67	6.58	7.38	6.33	7.15	29.82	29.94	16.51
80	12.62	10.77	6.69	6.67	6.58	7.38	6.34	7.16	29.82	29.94	16.51
90	12.62	10.78	6.69	6.67	6.58	7.39	6.34	7.16	29.82	29.94	16.51

Table 149 (continued)

Average C_v Over Range from 298 °K to T

(calories/mole/°K)

T, °K	CO_2	H_2O	CO	N_2	H_2	O_2	C(s)	HCl	Al_2O_3	B_2O_3	MgO
5900	12.63	10.78	6.69	6.67	6.59	7.39	[illegible]	7.16	29.82	29.94	16.52
10	12.63	10.78	6.69	6.67	6.59	7.39	6.34	7.17	29.82	29.94	16.52
20	12.64	10.79	6.69	6.67	6.59	7.39	6.35	7.17	29.82	29.94	16.52
30	12.64	10.79	6.69	6.67	6.59	7.40	6.35	7.18	29.82	29.94	16.53
40	12.64	10.80	6.69	6.67	6.59	7.40	6.36	7.18	29.83	29.94	16.53
50	12.64	10.80	6.70	6.68	6.59	7.40	6.36	7.18	29.83	29.94	16.53
60	12.65	10.81	6.70	6.68	6.60	7.40	6.36	7.19	29.83	29.94	16.54
70	12.65	10.81	6.70	6.68	6.60	7.40	6.36	7.19	29.83	29.94	16.54
80	12.65	10.82	6.70	6.68	6.60	7.41	6.37	7.19	29.84	29.95	16.54
90	12.66	10.82	6.70	6.68	6.60	7.41	6.37	7.20	29.84	29.95	16.55
6000	12.66	10.82	6.70	6.68	6.60	7.41	6.37	7.20	29.84	29.95	16.55
10	12.66	10.83	6.70	6.68	6.61	7.41	6.37	7.20	29.84	29.95	16.55
20	12.67	10.83	6.70	6.68	6.61	7.42	6.38	7.21	29.84	29.95	16.56
30	12.67	10.84	6.70	6.69	6.61	7.42	6.38	7.21	29.84	29.95	16.56
40	12.67	10.84	6.71	6.69	6.61	7.42	6.39	7.22	29.84	29.95	16.56
50	12.68	10.85	6.71	6.69	6.61	7.42	6.39	7.22	29.85	29.95	16.57
60	12.68	10.85	6.71	6.69	6.62	7.42	6.39	7.22	29.85	29.95	16.57
70	12.68	10.85	6.71	6.69	6.62	7.43	6.40	7.23	29.85	29.95	16.57
80	12.69	10.86	6.71	6.69	6.62	7.43	6.40	7.23	29.85	29.96	16.58
90	12.69	10.86	6.71	6.69	6.62	7.43	6.40	7.24	29.86	29.96	16.58
6100	12.69	10.87	6.71	6.69	6.62	7.43	6.40	7.24	29.86	29.96	16.58
10	12.70	10.87	6.71	6.70	6.63	7.44	6.41	7.24	29.86	29.96	16.58
20	12.70	10.88	6.71	6.70	6.63	7.44	6.41	7.25	29.86	29.96	16.59
30	12.70	10.88	6.71	6.70	6.63	7.44	6.41	7.25	29.86	29.96	16.59
40	12.70	10.88	6.72	6.70	6.63	7.44	6.42	7.26	29.87	29.96	16.60
50	12.71	10.89	6.72	6.70	6.63	7.44	6.42	7.26	29.87	29.96	16.60
60	12.71	10.89	6.72	6.70	6.64	7.44	6.42	7.26	29.87	29.96	16.60
70	12.71	10.90	6.72	6.70	6.64	7.45	6.43	7.27	29.87	29.96	16.60
80	12.72	10.90	6.72	6.71	6.64	7.45	6.43	7.27	29.88	29.96	16.61
90	12.72	10.91	6.72	6.71	6.64	7.45	6.43	7.28	29.88	29.96	16.61
6200	12.72	10.91	6.72	6.71	6.65	7.45	6.44	7.28	29.88	29.97	16.62
10	12.72	10.92	6.72	6.71	6.65	7.45	6.44	7.28	29.88	29.97	16.62
20	12.73	10.92	6.72	6.71	6.65	7.46	6.44	7.29	29.88	29.97	16.62
30	12.73	10.93	6.73	6.71	6.65	7.46	6.44	7.29	29.88	29.97	16.62
40	12.73	10.93	6.73	6.71	6.65	7.46	6.45	7.30	29.88	29.97	16.63
50	12.74	10.93	6.73	6.71	6.65	7.46	6.45	7.30	29.88	29.97	16.63
60	12.74	10.94	6.73	6.72	6.66	7.46	6.45	7.30	29.89	29.97	16.63
70	12.74	10.94	6.73	6.72	6.66	7.47	6.45	7.31	29.89	29.97	16.64
80	12.75	10.94	6.73	6.72	6.66	7.47	6.46	7.31	29.89	29.97	16.64
90	12.75	10.95	6.73	6.72	6.66	7.47	6.46	7.31	29.89	29.98	16.64
6300	12.75	10.95	6.73	6.72	6.67	7.47	6.46	7.32	29.90	29.98	16.65
10	12.76	10.96	6.73	6.72	6.67	7.47	6.47	7.32	29.90	29.98	16.65
20	12.76	10.96	6.73	6.72	6.67	7.47	6.47	7.32	29.90	29.98	16.65
30	12.76	10.97	6.74	6.72	6.67	7.48	6.47	7.33	29.90	29.98	16.66
40	12.76	10.98	6.74	6.73	6.67	7.48	6.48	7.33	29.90	29.98	16.66
50	12.77	10.98	6.74	6.73	6.68	7.48	6.48	7.34	29.91	29.98	16.66
60	12.77	10.98	6.74	6.73	6.68	7.48	6.48	7.34	29.91	29.98	16.67
70	12.77	10.99	6.74	6.73	6.68	7.48	6.48	7.34	29.91	29.98	16.67
80	12.78	10.99	6.74	6.73	6.68	7.48	6.49	7.35	29.91	29.98	16.67
90	12.78	11.00	6.74	6.73	6.68	7.49	6.49	7.35	29.91	29.98	16.67
6400	12.78	11.00	6.74	6.73	6.69	7.49	6.50	7.35	29.92	29.98	16.68
10	12.79	11.01	6.74	6.73	6.69	7.49	6.50	7.36	29.92	29.98	16.68
20	12.79	11.01	6.75	6.73	6.69	7.49	6.50	7.36	29.92	29.99	16.68
30	12.79	11.01	6.75	6.74	6.69	7.49	6.50	7.36	29.92	29.99	16.69
40	12.80	11.02	6.75	6.74	6.70	7.50	6.51	7.37	29.92	29.99	16.69
50	12.80	11.02	6.75	6.74	6.70	7.50	6.51	7.37	29.93	29.99	16.69
60	12.80	11.03	6.75	6.74	6.70	7.50	6.51	7.38	29.93	29.99	16.70
70	12.80	11.03	6.75	6.74	6.70	7.50	6.52	7.38	29.93	29.99	16.70
80	12.81	11.03	6.75	6.74	6.70	7.50	6.52	7.38	29.93	29.99	16.70
90	12.81	11.04	6.75	6.74	6.70	7.50	6.52	7.39	29.93	29.99	16.71
6500	12.82	11.04	6.75	6.74	6.71	7.51	6.52	7.39	29.94	29.99	16.71
10	12.82	11.05	6.75	6.74	6.71	7.51	6.53	7.40	29.94	30.00	16.71
20	12.82	11.05	6.76	6.75	6.71	7.51	6.53	7.40	29.94	30.00	16.72
30	12.82	11.06	6.76	6.75	6.71	7.52	6.54	7.40	29.94	30.00	16.72
40	12.83	11.06	6.76	6.75	6.71	7.52	6.54	7.41	29.94	30.00	16.72
50	12.83	11.07	6.76	6.75	6.72	7.52	6.54	7.41	29.95	30.00	16.73
60	12.83	11.07	6.76	6.75	6.72	7.52	6.54	7.42	29.95	30.00	16.73
70	12.84	11.07	6.76	6.75	6.72	7.52	6.55	7.42	29.95	30.00	16.74
80	12.84	11.08	6.76	6.75	6.72	7.52	6.55	7.43	29.95	30.00	16.74
90	12.84	11.08	6.76	6.75	6.73	7.53	6.56	7.43	29.95	30.00	16.74

Table 149 (continued)

Average C_v Over Range from 298 °K to T
(calories/mole/°K)

T, °K	CO_2	H_2O	CO	N_2	H_2	O_2	C(s)	HCl	Al_2O_3	B_2O_3	MgO
6600	12.84	11.09	6.77	6.76	6.73	7.53	6.56	7.43	29.96	30.00	16.74
10	12.85	11.09	6.77	6.76	6.73	7.53	6.56	7.43	29.96	30.00	16.75
20	12.85	11.10	6.77	6.76	6.73	7.54	6.56	7.44	29.96	30.00	16.75
30	12.85	11.10	6.77	6.76	6.73	7.54	6.57	7.44	29.96	30.00	16.76
40	12.86	11.10	6.77	6.76	6.74	7.54	6.57	7.44	29.96	30.00	16.76
50	12.86	11.11	6.77	6.76	6.74	7.54	6.57	7.45	29.97	30.01	16.76
60	12.86	11.11	6.77	6.76	6.74	7.54	6.57	7.45	29.97	30.01	16.77
70	12.86	11.12	6.77	6.76	6.74	7.55	6.58	7.46	29.97	30.01	16.77
80	12.87	11.12	6.77	6.77	6.74	7.55	6.58	7.46	29.97	30.01	16.77
90	12.87	11.12	6.77	6.77	6.75	7.55	6.58	7.46	29.97	30.01	16.78
6700	12.88	11.13	6.77	6.77	6.75	7.55	6.58	7.47	29.98	30.01	16.78
10	12.88	11.13	6.78	6.77	6.75	7.56	6.58	7.47	29.98	30.01	16.78
20	12.88	11.14	6.78	6.77	6.75	7.56	6.59	7.47	29.98	30.02	16.79
30	12.88	11.14	6.78	6.77	6.75	7.56	6.59	7.48	29.98	30.02	16.79
40	12.89	11.15	6.78	6.77	6.76	7.56	6.60	7.48	29.98	30.02	16.79
50	12.89	11.15	6.78	6.77	6.76	7.56	6.60	7.48	29.99	30.02	16.80
60	12.89	11.16	6.78	6.77	6.76	7.56	6.60	7.49	29.99	30.02	16.80
70	12.90	11.16	6.78	6.77	6.76	7.56	6.60	7.49	29.99	30.02	16.80
80	12.90	11.16	6.78	6.77	6.76	7.57	6.61	7.50	29.99	30.02	16.80
90	12.90	11.17	6.78	6.77	6.77	7.57	6.61	7.50	29.99	30.02	16.81
6800	12.91	11.17	6.78	6.78	6.77	7.57	6.61	7.50	30.00	30.02	16.81
10	12.91	11.18	6.78	6.78	6.77	7.57	6.62	7.51	30.00	30.02	16.81
20	12.91	11.18	6.78	6.78	6.77	7.58	6.62	7.51	30.00	30.02	16.82
30	12.92	11.19	6.79	6.78	6.77	7.58	6.62	7.52	30.00	30.02	16.82
40	12.92	11.19	6.79	6.78	6.78	7.58	6.62	7.52	30.00	30.02	16.82
50	12.92	11.20	6.79	6.79	6.78	7.58	6.63	7.52	30.01	30.03	16.82
60	12.92	11.20	6.79	6.79	6.78	7.58	6.63	7.53	30.01	30.03	16.83
70	12.93	11.20	6.79	6.79	6.78	7.58	6.63	7.53	30.01	30.03	16.83
80	12.93	11.21	6.79	6.79	6.79	7.59	6.64	7.53	30.01	30.03	16.83
90	12.93	11.21	6.79	6.79	6.79	7.59	6.64	7.54	30.01	30.03	16.84
6900	12.94	11.22	6.79	6.79	6.79	7.59	6.64	7.54	30.02	30.03	16.84
10	12.94	11.22	6.80	6.79	6.79	7.59	6.64	7.54	30.02	30.03	16.84
20	12.94	11.23	6.80	6.80	6.79	7.60	6.65	7.55	30.02	30.03	16.84
30	12.95	11.23	6.80	6.80	6.79	7.60	6.65	7.55	30.02	30.03	16.85
40	12.95	11.24	6.80	6.80	6.80	7.60	6.65	7.56	30.02	30.03	16.85
50	12.95	11.24	6.80	6.80	6.80	7.60	6.66	7.56	30.03	30.04	16.86
60	12.96	11.24	6.80	6.80	6.80	7.60	6.66	7.56	30.03	30.04	16.86
70	12.96	11.25	6.80	6.80	6.80	7.61	6.66	7.57	30.03	30.04	16.86
80	12.96	11.25	6.80	6.80	6.80	7.61	6.67	7.57	30.03	30.04	16.86
90	12.96	11.26	6.80	6.80	6.80	7.61	6.67	7.57	30.04	30.04	16.87

ratio, $\frac{a}{MW}$, is obtained. The molecular weight of the mixture may be calculated from the equation

$$MW_{mixture} = \frac{100}{\frac{a}{MW_1} + \frac{b}{MW_2}} \qquad (3)$$

where a and b are the weight per cents of the components and MW_1 and MW_2 their respective molecular weights. The molar ratios are then multiplied by the $\frac{MW_{mixture}}{100}$ to convert to the basis of one mole of mixtures as shown. The total number of carbon, hydrogen, nitrogen and oxygen atoms are added in the form provided on the reverse side and the detonation equation is written according to the rules set forth on page 580. The heat of combustion at constant volume (H_2O gas) is calculated as the sum of the heat of combustion of each component times its molar quantity. The heat of explosion, flame temperature, number of moles, MW_g and final power are then calculated in the same manner as that described for a pure compound.

Figures 90 and 91 represent a similar calculation for a metallized mixture, Torpex, illustrating Rule 4, page 580. This calculation shows the effect of considering the Al_2O_3 as solid and gaseous.

E. Conclusions and Recommendations

The application of this system to the calculation of some two hundred high explosives (pure compounds and mixtures) for which ballistic mortar values have been determined shows a reasonably good correlation between observed and calculated power values as expressed in per cent TNT.

This method of calculation has two major uses, (1) the preliminary evaluation of new compounds and mixtures without the necessity for making and testing them, and (2) the checking of observed data. These uses have been illustrated in the discussion.

The future extension of this system depends upon the availability of additional thermodynamic data, upon further studies of the reaction mechanisms involved in the explosive mixtures particularly those containing metals, and upon the retesting of those explosives for which the correlation between measured and calculated power is unsatisfactory.

The somewhat less satisfactory agreement achieved for the metallized mixtures (Table 145) leads to the conclusion that the observed values bear redetermination either in the ballistic mortar or the new-type spherical lead block. Rather than merely repeating the measurements already made, it is recommended that a program be laid out to include the investigation of

1. The optimum amount of aluminum for any one mixture;
2. The relative contribution to the power of high explosives of a number of metals, including among others aluminum, boron, beryllium, magnesium and lithium and possibly some of their hydrides;
3. The effect of the addition of high-nitrogen or other high energy compounds to metallized explosives; and
4. The relationship between the various test procedures including ballistic mortar, lead block, closed-blast and open-air blast.

The details of such a program must await the completion of a study on metallized explosives which is now underway.

In Table 148 there are listed pure compounds calculated to have powers in excess of 159% TNT, the highest so far measured or calculated for a known pure compound, MEDINA. It is recommended that if feasible, one or more of these compounds be synthesized and measured in the ballistic mortar and spherical lead block.

The large discrepancies existing between observed and calculated power for compounds of large positive oxygen balance, numbers 136, 240, 327 and 337 (Table 146) should probably be investigated further by a remeasurement of compounds 136 and 327 and any others of high positive oxygen balance which can be conveniently obtained.

F. References

1. Aerojet Engineering Corp., Report No. 512, Contract N7 onr-46208 by M. H. Gold and A. O. Dekker (14 June 1951). CONFIDENTIAL

2. J. S. Arthur, J. App. Phys., 21, 732 (1950). "The specific heats of MgO, TiO_2 and ZrO_2 at high temperatures".

3. Arthur D. Little, Inc., Contract W-19-020-ORD-6436 (2 January 1947). "Study of pure explosive compounds. Part I. Correlation of organic structure with explosive properties from existing data". CONFIDENTIAL

4. Arthur D. Little, Inc., Contract W-19-020-ORD-6436 (2 April 1947). "Study of pure explosive compounds. Part II. Correlation of thermal quantities with explosive properties". CONFIDENTIAL

5. Arthur D. Little, Inc., Contract W-19-020-ORD-12 (1 May 1950). "Study of pure explosive compounds. Part III. Correlation of composition of mixtures with performance". CONFIDENTIAL

6. Arthur D. Little, Inc., Contract W-19-020-ORD-6436 and DA-19-020-ORD-12 (1 March 1951). "Second report on synthesis and testing of high explosives". pp. 367-371. CONFIDENTIAL See also Arthur D. Little, Inc., "Fundamental research on high explosives. Abstract of work performed under contract DA-19-020-ORD-12 with Office of the Chief of Ordnance". (11 October 1950) CONFIDENTIAL

7. National Bureau of Standards, "Selected values of chemical thermodynamic properties. Series I and II". U. S. Dept. of Commerce, Washington, D. C. (30 June 1947).

8. Naval Ordnance Laboratory, "Report on the program to develop an improved HBX-type explosive". NavOrd Report 1502, 26 July 1950. CONFIDENTIAL

9. W. Nernst and K. Wohl, Zeitschr. f. techn. physik 608-614 (1929). "Specific heats at high temperature".

10. OSRD 547. J. O. Hirschfelder, F. T. McClure, C. F. Curtiss, and D. W. Osborne, "Thermodynamic properties of propellant gases". (23 November 1942) RESTRICTED

11. J. C. Southard, J. Am. Chem. Soc., 63, 3147 (1941). "The thermal properties of crystalline and glassy boron trioxide".

12. A. Thuret, J. Soc. Glass Tech., 20, 680-84 (1936). "Calculation of the specific heats of vitreous silica and components of glasses as functions of the temperature".

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